MODELING OF MECHANICAL PROPERTIES IN ALPHA/ BETA-TITANIUM ALLOYS

A Dissertation

Presented in Partial Fulfillment of the Requirements for
the Degree Doctor of Philosophy in the
Graduate School of the Ohio State University

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***

The Ohio State University,
2005

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The accelerated insertion of titanium alloys in component application requires the development of predictive capabilities for various aspects of their behavior, for example, phase stability, microstructural evolution and property-microstructure relationships over a wide range of length and time scales. In this presentation some novel aspects of property-microstructure relationships and microstructural evolution in α/β Ti alloys will be discussed. Neural Network (NN) Models based on a Bayesian framework have been developed to predict the mechanical properties of α/β Ti alloys. The development of such rules-based model requires the population of extensive databases, which in the present case are microstructurally-based. The steps involved in database development include producing controlled variations of the microstructure using novel approaches to heat-treatments, the use of standardized stereology protocols to characterize and quantify microstructural features rapidly, and mechanical testing of the heat-treated specimens. These databases have been used to train and test NN Models for prediction of mechanical properties. In addition, these models have been used to identify the influence of individual microstructural features on the mechanical properties, consequently guiding the efforts towards development of more robust mechanistically based models. In order to understand the property-microstructure relationships, a detailed understanding of...
microstructure evolution is imperative. The crystallography of the microstructure developing as a result of the solid-state $\beta \rightarrow \beta + \alpha$ transformation has been studied in detail by employing Scanning Electron Microscopy (SEM), Orientation Imaging Microscopy (in a high resolution SEM), site-specific TEM sample preparation using focused ion beam, and TEM based techniques. The influence of variant selection on the evolution of microstructure will be specifically addressed.
Dedicated to my Parents, Brother, Sister-in-law and all family members
ACKNOWLEDGEMENTS

First and foremost, I wish to express my sincere gratitude to my adviser, Prof. Hamish L. Fraser, who has been the continuous source of inspiration, encouragement and intellectual stimulations. I am grateful to him for letting me work on such an interesting topic, through which I could build both my computational and characterization skills. He has given an unwavering support with all kinds of equipments and computational tools. I really appreciate the confidence he had in me throughout my research work with him. His far-reaching vision, invaluable guidance and great support made this thesis possible.

I wish to thank Dr. Rajarshi Banerjee for his encouragement, inspiration and guidance throughout my stay in the Ohio State University. He has helped me in various ways in my work through his discussions and valuable comments in scientific research. He has also been a great friend, giving a great mental support in times of personal needs.

I like to thank all the members of Dr. Fraser’s research group for their invaluable help in various aspects of my research. I like to thank Dr. Babu Viswanathan and Dr. Dhriti Bhattacharyya for their valuable discussions and comments on my scientific research.

I like to thank Mrs Su Meng for helping me in sample preparation techniques. Su taught me many instruments, starting from EDM to Dual Beam FIB, which I have used
for my research. I am grateful to Mr. Garry Dodge for his help in the laboratory for furnace setup, calibration and other help.

I would like to thank Mrs Alison Polasik for her great help in proofreading my dissertation. Her valuable comments helped me make my dissertation document better.

I wish to express my deepest gratitude to my family. Whatever I have accomplished to date has been possible by the love, encouragement, and inspiration from my parents and my brother. My sister-in-law and all my relatives have given a tremendous support to me and to my family, making my accomplishments smoother and easier.
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CHAPTER 1

INTRODUCTION

Titanium alloys have been studied intensively over the last few decades due to their important technological applications. Their corrosion resistance, low density, high strength at elevated temperatures and good formability have prompted the use of these alloys in wide range of applications ranging from aircraft engine and structural components to bio-applications. Two phase $\alpha/\beta$ Ti alloys constitute the group which have the most diverse applications, including aircraft jet engine components, bicycle frames, orthopaedic and dental implants, golf clubs, etc.

The mechanical properties and application of these $\alpha/\beta$ titanium alloys appear to depend essentially on the characteristics of their microstructures. Therefore, a model to predict the mechanical properties of these alloys must relate microstructural features with properties. However the complexity of the microstructural features involved makes it rather difficult to develop a predictive model for mechanical properties in $\alpha/\beta$ titanium alloys. The microstructure is complex not only because it involves features which span a wide range of length scales, but also because those features are interdependent. It is not possible by any thermo-mechanical treatment to study the variation of only one
microstructural feature while holding the others at a fixed value and study its individual effect on properties.

Unfortunately, there has not been any physically based model developed to date capable of relating microstructural features to mechanical properties in α/β titanium alloys. Although the strengthening mechanisms of Ni-based, Al-based and steel alloys are well known and characterized by mathematical relationships, no mathematical relation is available to relate the microstructural features to mechanical properties in the case of titanium alloys. While many researchers have studied the influence of processing parameters on properties, there has been less emphasis on studies of the relationship of microstructural features with mechanical properties for these alloys. The current state of the art tool for relating microstructural features to the properties of these alloys is that proposed by Lutjering et. al.[1] where the experimentally observed microstructural influence on properties is indicated qualitatively by +(positive), -(negative) or 0 (no influence). There is a need for a more quantitative tool for prediction of microstructure/property relationships.

To build a microstructurally based quantitative predictive model for mechanical properties of α/β titanium alloys, a computational tool is required which can handle the challenges mentioned above. Artificial Neural Networks (ANN) are modeling tools that can handle a large number of variables with complex interdependencies without any prior knowledge of the physics of the problem. Their flexibility make them an attractive choice for developing a predictive model in a reasonable time frame.
In order to understand the property-microstructure relationships in these alloys a detailed understanding of microstructural evolution is imperative. When heat-treated in the $\beta$ phase field, the $\alpha/\beta$ titanium alloys develop the Widmanstätten microstructure. Typically, if the cooling rate following the heat treatment is relatively slow, a colony microstructure, consisting of groups of $\alpha$ laths belonging to the same crystallographic variant (colony), develops. In contrast, on employing faster rates when cooling from above the $\beta$ transus temperature, a basketweave microstructure develops. The basketweave microstructure consists of multiple variants of $\alpha$ laths clustered in the same region. Little is known about how the colony and basketweave microstructures form, despite the recognition that such microstructural details play a dominant role in determining the mechanical properties of these alloys. While previous work has investigated the formation of side-plates of $\alpha$ from the GB $\alpha$ precipitates, the selection of $\alpha$ variants and further growth of these side-plates during the solid-state transformation resulting in the contrast between the final microstructures (colony versus basketweave) has not been investigated in detail.

In the first part of this document microstructure evolution at different time and temperature scales will be discussed. Different crystallographic criteria for the nucleation & growth of colony and basketweave microstructure will be addressed.

The later part of this document will discuss the development of Neural Network Models based on a Bayesian framework to predict different mechanical properties of Ti-6Al-4V at room temperature. The different mechanical properties for which neural
network models have been developed are tensile properties (yield strength (YS), ultimate tensile (UTS) strength, elongation), fracture toughness, and creep properties.
CHAPTER 2

BACKGROUND AND LITERATURE REVIEW

2.1 Phases in Titanium Alloys:

2.1.1 Equilibrium Phases [2]:

Low temperature phase: $\alpha$ phase: It has a hexagonal close packed structure ($c/a = 1.587$) with two Ti atoms at (0,0,0) and (2/3, 1/3, 1/2). In pure Ti, the transition temperature for the $\alpha/\beta$ phase transformation is $\sim 883^\circ$ C. The elements Al, C, O, N, and Sn all stabilize the $\alpha$ phase by raising the $\alpha$ to $\beta$ transus temperature.

High temperature phase: $\beta$ phase: It has a body centered cubic structure with two Ti atoms at (0,0,0) and (1/2,1/2,1/2). The elements V, Mo, Cr and Cu all stabilize the $\beta$ phase by lowering the $\alpha$ to $\beta$ transition temperature.

$\alpha_{2\; \text{Ti}}\; 3\; \text{Al}$: It is an ordered phase, which is formed within $\alpha$ phase in alloys containing more than 6 wt% Al. The reaction is promoted by higher oxygen content.

$\gamma$-TiAl phase: It has an L1$_0$ structure with alternating (001) planes of Ti and Al. It is formed in alloys having a high Al content.
2.1.2 Non Equilibrium Phases[3]:

\textit{α′ - hexagonal martensite}: It is a supersaturated α phase with a fine lath morphology, and is produced by a diffusionless martensitic transformation upon rapid cooling from the β phase. It is more easily formed in alloys that are leaner in β stabilizing elements, because the \( M_s \) temperature decreases with an increase in β stabilizing elements. Morphologically, it is quite similar to lath α, although α’ martensite is more well-defined, generally thinner and has straight rather than curved sides.

\textit{α'' - Orthorhombic martensite}: It is another non-equilibrium phase formed by diffusionless transformations in certain alloys (there seems to be some confusion among researchers in this field as to the nomenclature of the two martensitic phases, they are often interchanged by different authors. See for example the paper by Williams and Blackburn [4] on Ti phase transformations and Non-equilibrium phases in Ti alloys handbook[5]).

\textit{ω phase}: It is a hexagonal phase and is supposed to be a transition phase during the formation of α from β. It occurs in near-β alloys and can lead to severe embrittlement. It can be induced by high hydrostatic pressures. It can also form within β of certain compositions either during quenching, as an athermal transformation product, or during aging in the form of ω precipitates.
2.2 **Titanium Alloying elements:**

Titanium alloying additions can be divided into two groups, $\alpha$ and $\beta$ stabilizers [6]. The $\alpha$ stabilizers can then be further subdivided into:

a) “Pure” $\alpha$ stabilizing elements which raise the $\beta$ transus (such as substitutional aluminum, gallium, germanium and interstitial oxygen) and,

b) “$\alpha$ strengthening” elements which have a high solubility in the alpha phase (such as tin and zirconium) but which do not raise the $\beta$ transus.

The amount of $\alpha$ stabilizer that can be added to titanium is restricted by $\alpha_2$, a coherent ordered phase based on Ti$_3$Al which causes embrittlement.

The $\beta$ stabilizing elements can also be subdivided into two groups. They include:

a) The $\beta$ isomorphous additions such as BCC elements Vanadium and Molybdenum which continuously lower the $\beta$ transus and

b) The $\beta$ stabilizing eutectoid formers such as iron and chromium which also lower the $\beta$ transus until this process is interrupted by compound formation.

Si is added to some titanium alloys to increase strength and creep resistance [7].

Table 2.1 summarizes the common alloying elements used in titanium alloys.

2.3 **Classification of Titanium Alloys:**

The type and amount of alloying elements determines the amount of phases present at low temperatures. In discussing the metallurgy of titanium, it is common to separate the
alloys into three categories, referring to the relative amount of phases present at room
temperature. The alloy categories are: a) α alloys, b) β alloys and c) α/β alloys.

2.3.1 α alloys: Unalloyed titanium and Ti alloys with α stabilizers such as
aluminum, gallium and tin, are classified as α alloys. e.g. Ti-5Al-2.5Sn. They have α as
their stable phase at low temperatures. These alloys are characterized by satisfactory
strength, toughness, creep resistance, and weldability. Furthermore, the absence of a
ductile-brittle transformation, a property of the bcc structure, renders α alloys suitable for
cryogenic applications. However, they cannot be strengthened by varying the heat
treatment because the α phase is stable. The only ways to strengthen α alloys are a) Cold
work, b) cold work followed by annealing to control α grain size and c) solution
strengthening.

α alloys which contain small amounts (about 1 to 2 %) of β stabilizers have been
classified as “near-alpha” alloys. Since the near-alpha alloys contain some β stabilizers,
these can exhibit microstructural changes similar to those in the α/β alloys. However,
these alloys are composed primarily of the α phase and will behave more like the α alloys
than the α/β alloys in their response to heat treatment and age hardening.

2.3.2 β alloys: β alloys are formed with large amounts of β-stabilizers which
lower the α-β transition temperature (See figure.2.1[8]). Some important β alloys are Ti-
10V-2Fe-3Al, Ti-15V-3Cr-3Al-3Sn, etc. Beta alloys are extremely formable. They are,
however, prone to ductile-brittle transformation and hence unsuitable for low
temperature applications. These alloys generally provide increased fracture toughness over α/β alloys at a given strength level.

2.3.3 α/β alloys: The α/β alloys at equilibrium contain a mixture of α and β phases. They contain mixtures of both α and β stabilizers. They combine the strength of α alloys with the ductility of β alloys, and their microstructure and properties can be varied widely by appropriate heat treatments and thermomechanical processing.

2.4 Thermomechanical Processing and Microstructure Evolution:

The distribution and morphology of the α and β phases depend on processing history and can be manipulated extensively both by heat treatment and by thermomechanical processing (TMP).

2.4.1 Microstructure variation with thermal treatment alone:

When an α/β Ti alloy sample is heated to a temperature above the β transus, the whole sample is transformed to β. If the alloy is kept at this temperature for too long or taken to too high a temperature, there may be excessive grain growth of β, which should be avoided. A typical β-processing heat treatment schedule is shown schematically in figure 2.2 [9]. Cooling down from the homogenizing temperature to room temperature will yield a new microstructure following phase transformation. This transformation can occur by nucleation & growth (N & G) or it can occur martensitically, depending upon the alloy composition and cooling rate. The effect of cooling rate on the constitution of an α/β alloy is shown schematically in the continuous cooling transformation (CCT) diagram shown in figure 2.3[10].

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In general, the C-curve for the $\beta$ to $\alpha+\beta$ N & G transformation moves to the right as the $\beta$ stabilizer concentration increases. Alloys which contain enough $\beta$ stabilizing elements to depress the $M_s$ temperature below room temperature can be rapidly cooled to retain the metastable $\beta$ phase, which is usually transformed to an $\alpha + \beta$ mixture during a subsequent isothermal aging treatment. The resulting microstructures that correspond to martensitic and N & G transformation are shown in figure 2.4[10].

The $\alpha'$ structure consists of an acicular hcp martensite which is supersaturated in $\beta$-stabilizing elements such as V or Mo. The N & G structure consists of colonies of $\alpha$ laths which are separated by thinner laths of $\beta$ phase. Both the $\alpha'$ and the N & G $\alpha$ have the Burgers orientation relationship with respect to the parent $\beta$ phase. The Burgers OR is $\{0001\}_\alpha || \{110\}_\beta$ and $<1\bar{1}20> _\alpha || <1\bar{1}1> _\beta$. There are 12 crystallographic variants of this relationship. The martensitic structure is always finer, and the individual plates are more randomly oriented than in the N & G structure.

An additional feature that can be seen in most alloys that have been cooled from above the $\beta$ transus is grain boundary $\alpha$ (GB $\alpha$). Grain-boundary $\alpha$ is heterogeneously nucleated at prior $\beta$ grain boundaries. Examples of grain boundary $\alpha$ are shown in figure 2.5. The thickness and continuity of this layer depends on cooling rate and alloy composition. The relative kinetics of GB and inter-granular $\alpha$ formation are schematically represented in the CCT diagram, figure 2.6 [10].

2.4.2 Microstructure variation with thermomechanical processing:
The effect of thermomechanical processing (TMP) on the microstructure is also very pronounced. If an \( \alpha/\beta \) alloy is forged in the \( \alpha+\beta \) phase field, and then annealed below the \( \beta \) transus, the phase may undergo recrystallization and globularization depending on the amount of deformation it has received. In general, the greater the amount of deformation, the greater the fraction of the recrystallized and globularized material.\[11\] It was found that a critical amount of deformation (minimum true strain) is required to cause substantial globularization of \( \alpha \) laths so that the aspect ratio of these laths could be of the order of 1-3 \[12\]. A typical processing procedure for an \( \alpha/\beta \) forging treatment is shown schematically in figure 2.7 \[9\].

Globularization may occur by two different mechanisms. The first one involves the pinching off of the \( \alpha \) phase by the \( \beta \) phase at the interface between two adjacent recrystallized \( \alpha \) crystals and the neighboring \( \beta \) lath. The \( \beta \) phase penetrates the boundary between the two recrystallized grains because a 180° dihedral angle is not permitted by the surface tension requirements and eventually separates them. The second mechanism involves regions of intense shear bands within the \( \alpha \) laths, which again form an \( \alpha/\alpha \) interface in contact with a \( \beta \) lath. There, too, surface tension causes a curvature in the \( \alpha/\beta \) interface and the \( \beta \) phase penetrates the boundary between the two sides of the \( \alpha \) crystal across the shear bands and separates them in two crystals, see figure 2.8 \[12\].

The recrystallization temperature and cooling rate also affect the final microstructure. In general, a higher recrystallization temperature will result in a lesser fraction of recrystallized equiaxed \( \alpha \), and a greater the amount of transformed \( \beta \).
Similarly the slower the cooling rate from the recrystallization temperature, the more the equiaxed α grains will grow at the cost of the α lamellae[9].

Lütjering[9] listed important processing parameters and resulting microstructural features for both the β solution treatment and TMP at α+β region. They are shown in tables 2.2 and 2.3.

There has been some progress made in understanding the use of TMP in refining α grain size in alloys such as Ti-6Al-4V [13]. The central idea in this work is that the recrystallized primary α grain size is directly related to the dimensions of the α-phase regions which are subjected to deformation and recrystallization. Thus, in Ti-6Al-4V, for example, rapid cooling from above the β transus to refine the α plate size, followed by reheating in the α+β region and forging with fairly heavy deformations, permits the recrystallized α grains, 1 to 2 μm in diameter, to be achieved during annealing at ~800°C. This is a useful way to produce very fine grain size; however, the necessary refinement of the scale of the β to α+β microstructure requires high cooling rates, and this in turn requires small section size [10].

TMP is also an effective means of controlling grain boundary α formation. Continuous working down through the transus introduces alternate heterogeneous nucleation sites in the form of dislocations that the role of β grain boundaries as the sole heterogeneous nucleation sites is considerably reduced.

2.4.3 Sequence of phase transformations in α/β Ti alloys during continuous heating:
When a microstructure consists of globular primary $\alpha$ and a mixture of $\alpha$ and $\beta$ laths (transformed $\beta$), and it is heated slowly through the $\alpha/\beta$ region to above the $\beta$ transus, the transformation takes place in two steps. Sha et al.[14] observed this sequence by using Differential Scanning Calorimetric (DSC) studies, in which a Ti-6Al-4V specimen was heated at a constant rate. First, at a relatively low temperature below the $\beta$ transus, the $\alpha$ laths in the transformed $\beta$ start to transform to the $\beta$ phase. This corresponded to a peak in the heat flux vs. temperature curve. The second step, i.e. the transformation of primary or globular $\alpha$ into $\beta$, starts at a higher temperature and is almost completed when the temperature reaches the $\beta$ transus. This phenomenon is evident from a second peak in the same heat flux vs. temperature curve. The above experiments confirm the theoretical expectations, as it is known that the primary $\alpha$ that forms first while cooling has a lower $\beta$ stabilizer concentration than the $\alpha$ in the transformed $\beta$ due to the alloy partitioning effect. Therefore, the primary $\alpha$ is expected to have a higher transformation temperature. Further heating above the $\beta$ transus causes grain growth in the $\beta$ phase.

2.5 Microstructure Evolution in alloy Ti-6Al-4V:

Ti-6Al-4V is the most commonly used $\alpha+\beta$ alloy, having modest quantities of both alpha stabilizer (aluminum) and beta stabilizer (vanadium) and thereby combining reasonable strength with good formability. It finds uses in aerospace applications,
pressure vessels, aircraft turbine and compressor blades and disks, surgical implants etc. The microstructure evolution of Ti-6Al-4V has been studied in detail [15].

When Ti-6Al-4V is heated above 600°C, $\alpha$ starts transforming to $\beta$, and, the entire microstructure is composed of equiaxed $\beta$ grains above 995°C (beta transus temperature). When this alloy is slowly cooled from the $\beta$ region, $\alpha$ begins to form below the $\beta$ transus. The $\alpha$ forms in plates, having the Burgers OR with the $\beta$ in which it forms. Upon slow cooling, a nucleus of $\alpha$ forms and, because of the close atomic matching along this common plane, the $\alpha$ phase thickens relatively slowly perpendicular to this plane but grows faster along the plane, thus developing a lath-like structure consisting of $\alpha$ plates. The formation of $\alpha$ upon cooling is shown schematically in figure 2.9[15].

For most applications, Ti-6Al-4V is used in the $\alpha+\beta$ processed condition (which causes recrystallization and globularization as described before) followed by a single stage annealing process. If necessary, however, additional strength can be obtained by an $\alpha+\beta$ heat treatment. Figure 2.10 shows examples of the $\beta$ processed and $\alpha+\beta$ processed microstructures of Ti-6Al-4V.

2.6 Comparison Of Two Microstructures In Ti-64 With Respect To Mechanical Properties:

The mechanical properties of Titanium alloys can be varied over a wide range by thermomechanical treatments, producing a range of microstructures from bimodal to fully lamellar [16, 17]. While the bi-modal microstructures are reported to have advantages in
terms of yield stress, tensile ductility, and fatigue strength, fully lamellar structures are preferred for applications where high cycle fatigue crack propagation resistance, fracture toughness, and creep resistance are needed [18, 19]. Following are the advantages of bimodal and Widmanstätten microstructures.

2.6.1 Bimodal:

- Higher Ductility and formability
- Higher threshold stress for hot salt stress corrosion
- Higher strength (for equivalent heat treatment)
- Better hydrogen tolerance
- Better low-cycle fatigue (initiation) properties

2.6.2 Widmanstätten or Acicular:

- Superior creep properties
- Improved fatigue resistance and high values of toughness

Bimodal structure containing both globular and Widmanstätten features combine the advantages of both types of microstructures. For low temperature applications and small section sizes (<4”), α+β processed alloys are preferred because of their better LCF, tensile strengths and ductility [6].

Work done by Ashton et al. [20] indicates that the Widmanstätten type of microstructures, particularly those formed by fairly fast cooling rates from the “all beta “
region, give the best creep resistance and the highest room temperature tensile strength with satisfactory impact and fatigue resistances. However, the tensile ductility of specimens containing entirely Widmanstätten $\alpha$ is found to be low due to the finer structure.

2.7 Important Microstructural Parameters And Their Effects On Tensile Properties:

The properties of Ti alloys are strongly dependent on their microstructures, which in turn depend on heat treatment and thermomechanical processing. Therefore, many researchers have focussed on identifying the microstructure-property relationship. Table 2.4 [21] shows the influence of microstructural parameters on mechanical properties of $\alpha+\beta$ Ti-alloys. In the table, the author indicated the experimentally observed influence qualitatively by + (positive), - (negative), or 0 (no influence).

2.7.1 Lamellar structure:

According to Lütjering, Albrecht and Ivasishin [22] the critical microstructural parameters for fully lamellar structures with respect to mechanical properties are the $\beta$ grain size, the colony size, the width of the lamellae, and the character of the interlamellar interface. They cited grain boundary alpha, which can be considered as a continuous, thin soft layer along prior beta grain boundaries, as another important factor with respect to mechanical properties. They compared the property response of conventionally $\beta$ processed Ti alloy samples having large prior $\beta$ grains to that of a Ti alloy with smaller prior $\beta$ grains obtained by rapid heating methods. They showed that, while prior beta grain size has little or no influence on the yield stress (see figure 2.11[23]), it has a strong influence on ductility. They explained this dependence of
ductility on prior \( \beta \) grain size in the following way. The length of the \( \beta \) grain boundary limits the maximum slip length in the grain boundary \( \alpha \) layer; therefore, the stress concentration at grain boundary triple points is reduced for small \( \beta \) grain size, resulting in a higher ductility for smaller \( \beta \) grain.

According to Lütjering [1], the microstructural parameter which has the greatest influence on the mechanical properties of fully lamellar structures is the \( \alpha \) colony size. This is limited by the size of the prior \( \beta \) grain size. Lütjering observed that, with increasing cooling rate, the yield stress increases initially very slowly but above a certain cooling rate it increases drastically.

He explained the phenomenon solely in terms of the colony size factor. The colony size determines the effective slip length, and thus an increase in cooling rate will effectively reduce the slip length. This will in turn cause the yield stress to increase. A drastic increase in yield stress is observed when the colony structure is changed to a martensitic type of microstructure (slip length and colony size equal to the width of the individual \( \alpha \) plates).

However it must be acknowledged that this hypothesis that the variation of yield stress is solely due to changes in colony size is just a speculation, as we know that the cooling rate changes the microstructure in a complex way, not only affecting the colony size, but also the size and morphology of the other microstrutural features, such as the thickness of Widmanstätten alpha, width of grain boundary alpha layer etc. As it is not possible to use experimental methods to obtain a physical picture of the dependence of a
certain property on a single parameter, this type of physical model relating a property to a particular parameter is just a proposition.

Lütjering et al.[24] studied the variation of ductility with cooling rate. In contrast to the yield stress, which increases continuously with increasing cooling rate, the response of the ductility to changes in the cooling rate is more complex: it reaches a maximum at intermediate cooling rates. As the cooling rate increases beyond the maximum, the ductility decreases sharply. This observed behavior is believed to be the result of two competing effects. One contribution is the reduction of slip length by increasing the cooling rate; this reduces the pile-up length and decreases the stress concentrations, thereby delaying crack nucleation which results in higher ductility. However, while the lamellar structure is refined by increasing the cooling rate, the strength of the matrix increases until the strength difference between the matrix and the coarser α-layers along the β-grain boundaries is large enough to cause preferential deformation of the softer grain boundary α, which in turn leads to premature crack nucleation. The evidence for this change from transgranular to intergranular fracture is found on the fracture surfaces.

Boyer and Wallem[25] attempted to correlate the microstructural features of β-annealed Ti-6Al-4V at different conditions with tensile strength and ductility. However, they were unable to establish any correlation between prior β grain size, colony size or α plate width. They suggested that the relationship between tensile properties and microstructure must be determined by a complex combination of the individual parameters. A similar observation was made by Rhodes, et al.[26] when attempting to
establish a correlation of microstructural features to fatigue crack growth rate (FCGR). Boyer and Wallem[25] also studied the effect of cooling rate on the properties of β-annealed Ti-6Al-4V. They found that an increase in cooling rate is associated with an increase in tensile and yield strength with no consistent ductility correlation. The correlation of higher strengths with faster cooling rates is explained as that the faster cooling rates would result in a finer transformed structure leading to higher strength.

Ambard et al.’s work [27] on deformation mechanisms in Ti-6Al-4V indicates that a colony behaves as a single grain within which only the basal system is activated, while many glide systems can be activated in globular grains. They argued this is the reason behind the α colonies being more detrimental to ductility than globular grains. According to them, many dislocations of the same nature pile-up against colony boundaries and produce a high stress concentration during the deformation of colonies. As a consequence, damage is expected to nucleate at colony boundaries. They suggest that the colony size is an important microstructural parameter as far as ductility is concerned.

2.7.2 Bimodal structures:

For the bimodal structure, Lütjering[9] suggested that prior β grain size (limiting the colony size) and volume fraction of primary α are the most influential parameters on mechanical properties. A small β grain size in the bimodal microstructure leads to a small α colony size, and therefore to a short slip length. According to him, if the slip length were to be the the primary considerator, the bimodal microstructure should exhibit a higher yield stress, a higher ductility, a higher HCF strength, a slower crack propagation
rate of microcracks and a higher LCF strength as compared with a fully lamellar microstructure.

Lütjering mentions the alloy partitioning effect in bimodal structure, which he thinks is an important parameter for the mechanical properties of this microstructure. During the formation of primary $\alpha$ in the $\beta$ grains, those alloy elements which are either strong $\alpha$-stabilizer or strong $\beta$-stabilizer partition respectively into the two phases. Alloy element partitioning increases with $\alpha_p$ (primary $\alpha$) volume fraction. This effect leads to a lower basic strength within the lamellar part of the bimodal microstructure compared with a fully lamellar structure. The author observed a maximum in Y.S vs $\alpha_p$ volume fraction curve at 10-20 vol. % of $\alpha_p$. He explained this phenomenon by the two counteracting effects (increasing alloy element partitioning and decreasing colony size) caused by increasing $\alpha_p$ volume fraction. He concluded that for a small volume fraction of $\alpha_p$, the colony size effect is dominant, thereby increasing yield strength by lowering the colony size, and that for large volume fractions of $\alpha_p$ the alloy element partitioning effect dominates, which decreases the strength of the $\alpha$ lamellae in the bimodal structure.

Lütjering might be correct in his proposition, but the Ti alloy system is not so simple that one may be able to explain a phenomenon by only two parameters, instead, there are many other microstructural features changing simultaneously, each of which may affect the YS in a different way.
Ashton et al.[20] studied the tensile strength, elongation and reduction in area variation with % primary alpha in the α+β forged Hylite 50 and IMI 679 alloys. They found out that Hylite 50 results show an increase in the proof stress and tensile strength values with a corresponding fall in percentage elongation and particularly in reduction of area with decreasing primary α. In contrast, the IMI.679 results show a reduction of all properties as the percentage of primary alpha present in the microstructure is decreased. See figure 2.12[20].

The authors believed the behavior of strengthening with concomitant lowering of ductility, associated with decreasing amount of primary alpha in the microstructures to be due to the colony disposition of the stronger, close packed hexagonal α phase breaking up the continuity of and isolating the weaker β phase. The authors couldn’t advance any positive theory for the strengthening behavior of IMI.679 with increasing amount of primary alpha.

However, the theory advanced by Ashton and Chambers is deceptive; while they studied the variation of properties with amount of primary alpha, they did not consider any associated changes in other microstructural features (like colony size, alpha lath thickness, etc.). They seem to have assumed that the other microstructural parameters remain constant while changing only the percentage of primary alpha, but it is physically impossible to vary only one microstructural feature in Ti alloys while keeping others constant.
2.8 **Deformation Mechanisms And Slip Systems In Ti Alloys:**

The flow mechanisms and kinetics are different in the α and β phases in Ti-6Al-4V alloy. This results in a large number of deformation mechanisms responsible for the macroscopic behavior of the alloy. Their identification is crucial for understanding the mechanical response of this material.

According to M. J. Philippe[28], deformation in titanium alloys can be accomplished by gliding, twinning, and/or stress induced phase transformations. The selection of the different mechanisms activated during plastic deformation depends on the alloying elements, grain size, grain orientations and the test conditions (T, ε). The conditions of deformation modify the appearance of the mechanisms, eg., twinning is facilitated by low temperature and high strain rate. Philippe and other authors studied the effect of alloying elements on deformation mechanisms. Increasing the aluminum or oxygen content tends to impede twinning [29, 30, 31] and therefore, only glide mechanisms were found to be active in the alloys with a high level of aluminium and oxygen. An increase in the grain size increases in the twinning activity. Similarly [28], the grain shape has an influence on the twinning system activated during deformation.

Harold Margolin [32] made a significant contribution to the analysis of slip and twinning across α/β interfaces in titanium alloys in his paper with S.Ankem by taking into account the elastic interactions that occur at the interfaces in Widmanstätten or martensitic α/β interfaces. He demonstrated which slip systems are likely to be initiated.

S.J. Lecomte[33] in his work on plastic deformation of Ti-6Al-4V showed that, at room temperature, most dislocations are <a> type on the prismatic planes. Secondary slip
systems are basal or pyramidal \(\{\bar{1}01\}\). In the range of 230° C to 430° C, some of these so-called secondary slip systems are found to be the most active for dislocation motions; specifically \(<c+a>\) dislocation gliding on the pyramidal planes \(\{\bar{1}01\}\) and \(\{1\bar{2}2\}\) are prominent. At higher temperatures, prismatic slip is the common glide but cross-slip is very frequent.

Ambard et al.[27] investigated the deformation mechanisms of Ti-6Al-4V alloy at room temperature and cryogenic temperature using Atomic Force Microscopy and Transmission Electron Microscopy. They found that the nature of \(\alpha\) slip systems depends on the \(\alpha\) grain morphology. In globular grains, the main slip systems are prismatic as commonly observed in Ti alloys. On the basis of the Peierls-Nabarro model, prism slip is expected to replace basal slip as the predominant slip mode when the c/a ratio becomes <1.73, since then both the \(\{101\}\) spacing and density are greater than corresponding values for the basal plane.

However, the basal slip system is activated within colonies. This difference is attributed to the presence of the \(\beta\) phase between laths. The \(\frac{1}{3} < 2\bar{1}10 > (0001)\alpha\) slip system is parallel to the \(\frac{1}{2} < 111 > \{110\}\) slip system in the \(\beta\) phase. According to the authors, since the mismatch between \(\frac{1}{3}\left[\begin{array}{c} 2 \bar{1}10 \end{array}\right]_\alpha\) and \(\frac{1}{2}[111]_\beta\) burgers vectors is small (2%) and can be relaxed by the passage of about 50 dislocations, the transmission of the
deformation through the $\alpha/\beta$ interphase of this slip system should be relatively easy. The easy slip transmission of the basal system makes the colony size an important microstructural parameter compared to the $\alpha$ lath size. Jones et. al’s [34] work on stress-state dependence of slip in Ti-6Al-4V indicates that, $<a>$ dislocations can glide with almost equal ease on prismatic, basal and pyramidal planes.

2.9 **Application Of Neural Network In Materials Science[31]:**

Artificial neural networks (ANN) modeling is one of the most powerful modeling techniques available to the researchers today. In the cases where the problem is very complex and simplification is unacceptable, neural network models are thought to be extremely useful. These models are suitable for simulation of correlations which are hard to describe by physical models. There are highly complex problems in materials science where ANN is useful and in the past few years many researchers have tried to apply ANN modeling techniques in different fields of materials science.

2.9.1 **ANN in the field of Welding:**

Welding has seen major applications of the neural network method. Examples include: weld seam tracking where the output from sensors is interpreted by a trained network to control a welding robot [35]; the interpretation of sensor information measured during welding to determine weld quality[36, 37]; the detection of defects in welds using ultrasonic, radiation or other signals[38]; the estimation of weld profile (including penetration) from variations in welding parameters or other sensed
parameters[39]. The use of neural network is therefore well established in the control and monitoring of welds.

**Toughness:** The toughness of ferritic steel welds has been studied using neural networks [40]. The Charpy toughness was expressed as a function of the welding process (manual metal arc or submerged arc), the chemical composition (C, Mn, Si, Al, P, S, O & N), the test temperature and the microstructure (primary, secondary, allotriomorphic ferrite, Widmanstätten ferrite and acicular ferrite). The welding process was numerically distinguished in the analysis by using 0 and 1 for the manual and submerged arc methods. The authors used the existing literature data for generating their training database; the inclusion of microstructure greatly limited the quantity of data available for analysis because few such results are reported in the literature.

**Hardness:** Chan et al. [41] created a model for the hardness of the heat affected zone of steel welds as a function of the carbon concentration, the carbon-equivalent and the cooling rate within a specified temperature range. Having produced the model, they did not go further to investigate how the hardness depends on each of the input parameters, whether the relationship differs for low and high carbon steels, etc.

**Strength:** Svensson [42] has compiled an extensive list of linear regression equations for estimating the strength as a function of the weld metal chemical composition. The equations are limited to specific alloy systems and cover no more than five alloying elements. There is no facility for estimating the effect of heat treatments.

Cool et al have created a more generally applicable neural network model [43] using data from 1652 experiments reported in the published literature. One feature of the
analysis was that Cool et al. Used a committee of best models to make predictions. It is possible that a committee of models can make more reliable predictions than an individual model [44].

**Weld Cooling Rate:** In the study of the weld cooling rate problem, Chan et al. [45] used the inputs indicated by Adams’ Physical model and incorporated them into a neural network model to obtain a single model for all dimensionalities of heat flow. They demonstrated that the accuracy achieved is better with the neural network, given the approximations inherent in the analytical equations of Adam’s theory. One difficulty of their model is that it does not give error bars, which are dependent on the local fit so that the actual range of applicability is not clear. The reliability of the model is not established when extrapolated or interpolated beyond the domain of training data set.

### 2.9.2 ANN in the field of Superalloys:

The yield and ultimate tensile strength of nickel-base superalloys with $\gamma/\gamma'$ microstructures has been modeled [46, 47] using the neural network method, as a function of the Ni, Cr, Co, Mo, W, Ta, Nb, Al, Ti, Fe, Mn, Si, C, B and Zr concentrations, and of the test temperature. The analysis is based on data selected from the published literature.

**Fatigue properties of superalloys:** Fujii et al. [48] applied the neural network method to predicting fatigue properties. They have identified some 51 variables that could be expected to influence the fatigue crack growth rate in nickel base superalloys. Using the model, they studied the effect of each variable in isolation. They produced
some interesting results; for example, it was verified that an increase in the grain size should lead to decrease in fatigue crack growth rate when the grain size is varied without affecting any other input. This cannot be done in any experimental approach because the change in grain size is achieved by altering the heat treatment, which in turn influences other features of the microstructure.

*Fatigue threshold:* In a recent study of the fatigue thresholds in nickel-base superalloys, Schooling *et al.* have attempted to compare a “neurofuzzy” modelling approach with the classical neural network [49]. The application of the fuzzy rules to the network involves the biasing of the inputs according to human experience.

It was suggested that the fuzzy method has an advantage with restricted datasets because the complexity of the relationships can be restricted by the operator. This conclusion is surprising because the complexity of a classical network, when assessed for generalization, naturally tends to be minimized for small datasets.

Schooling *et al.* found it necessary to make significant adjustments to the fuzzy rules in order to reduce the mean square error to a value comparable to the classical network. This is evident that considerable operator bias is introduced in designing fuzzy networks. This may not be satisfactory for complex problems where the actual relationships are not understood to begin with.

The comparison of the two methods by Schooling *et al.* does not seem justified because the predictions of neurofuzzy method were not accompanied by error bars (other than the mean square error).
**Creep of superalloys:** Sathyanarayanan et al. [50] have developed a neural network model for the “creep feed grinding” of nickel-base superalloys and titanium alloys, using the feed rate, depth of cut and wheel bond type as inputs, and the surface finish, force and power as outputs.

**Lattice parameters of superalloys:**

The lattice constants of the \(\gamma\) and \(\gamma'\) phases of nickel superalloys have been modelled using a neural network within a Baysian framework [51]. The lattice parameters of the two phases were expressed as a nonlinear function of eighteen variables including the chemical compositions and temperature. It was possible to estimate the uncertainties and the method has proved to be extremely useful in understanding both the effect of solutes on the lattice mismatch, and on how this mismatch changes with temperature.

2.9.3 ANN in studying transformations:

**Continuous cooling transformation:** The transformation of austenite as the temperature decreases during continuous cooling has been modeled with the neural network method using the chemical composition, the austenisation temperature and cooling rate as inputs [52]. The results were concluded to be satisfactory but had large errors particularly for the bainite reaction. These large errors were attributed partly to noise in the experimental data, to the neglect of austenite grain size as an input, and to the assumption that all transformations occur at all cooling rates, whereas this is not the case in practice.
2.9.4 ANN in Steel processing and mechanical properties:

*Hot rolling:* Singh *et al.* [53] have developed a neural network model in which the yield and tensile strength of the steel is estimated as a function of some 108 variables, including the chemical composition and an array of rolling parameters. A similar model by Korczak *et al.* [54] uses microstructural parameters as inputs and has been applied to the calculation of the ferrite grain size and property distribution through the thickness of the final plate.

*Mechanical properties:* There are many examples of the use of neural networks to describe the mechanical properties of steels; Dumortier *et al.* have modeled the properties of microalloyed steels [55]; Millykoski [56, 57] has addressed the problem of strength variations in thin steel sheets; studies have been done on the microstructure-property relationship of C-Mn steels [58]; the tensile properties of mechanically alloyed iron have been analyzed and compared with predictions using physical models [59, 60].

2.9.5 ANN in the field of Polymeric & Inorganic Compounds:

Neural network methods have been used to model the glass transition temperatures of amorphous and semi-crystalline polymers to an accuracy of about 10K, and similar models have been developed for relaxation temperatures, degradation temperature, refractive index, tensile strength, elongation, notch strength and hardness [61, 62, 63].
2.9.6 ANN in the field of thin films & superconductors:

Neural networks have been used to interpret Raman Spectroscopy data to deduce the superconducting transition temperature of YBCO thin films during the deposition process [64], to characterize reflection high-energy electron diffraction patterns from semiconductor thin films in order to monitor the deposition process [65], to rapidly estimate the optical constants of thin films using the computational results of a physical model of thin films [66].

2.9.7 ANN in the field of Titanium Alloys:

There has been limited work on the application of neural networks in the field of titanium alloys. Malinov et al.[67] has used the neural network to determine the influence of alloying elements on transformation kinetics in titanium alloys. They simulated the time temperature transformation curve of different titanium alloys. In another work, Malinov et al.[68] designed a neural network for the prediction of the mechanical properties of titanium alloys as a function of the processing parameters and alloy composition. Their approach was not purely quantitative regarding the heat treatment. In the model they did not take into account the particular heat treatment parameters such as temperature of heating, time, heating/cooling rates etc. They assumed that all the heat treatment conditions were at optimal values for the corresponding heat treatment procedure and alloy. This assumption is not valid because they collected data from different literature sources in which the heat treatment parameters almost certainly varied.
Also, the authors did not consider the microstructural features, which affect the properties directly. Thus, their mechanical property model cannot be considered accurate.
Table 2.1: Common alloying elements used in titanium alloys

<table>
<thead>
<tr>
<th>α-stabilizing</th>
<th>β-isomorphous</th>
<th>β-eutectoid</th>
<th>Neutral</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>V</td>
<td>Cu</td>
<td>Zr</td>
</tr>
<tr>
<td>Ge</td>
<td>Nb</td>
<td>Ag</td>
<td>Hf</td>
</tr>
<tr>
<td>Ga</td>
<td>Ta</td>
<td>Au</td>
<td>Sn</td>
</tr>
<tr>
<td>La</td>
<td>Mo</td>
<td>In</td>
<td></td>
</tr>
<tr>
<td>Ce</td>
<td></td>
<td>Pb</td>
<td></td>
</tr>
<tr>
<td>O</td>
<td></td>
<td>Bi</td>
<td></td>
</tr>
<tr>
<td>N</td>
<td></td>
<td>Cr</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td></td>
<td>W</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Mn</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Fe</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Cu</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Ni</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Si</td>
<td></td>
</tr>
</tbody>
</table>

Table 2.2: Important processing parameters and resulting microstructural features, for fully lamellar microstructures

<table>
<thead>
<tr>
<th>Step</th>
<th>Important Parameters</th>
<th>Microstructural Features</th>
</tr>
</thead>
<tbody>
<tr>
<td>Homogenization in the β phase field</td>
<td>Temperature, Cooling Rate</td>
<td>Large β grain size, α lamellae size, Colony Size, GB α layer</td>
</tr>
<tr>
<td>Aging at α+β phase field</td>
<td>Aging temperature</td>
<td>Ti,Al in α, Secondary α in β</td>
</tr>
</tbody>
</table>
Table 2.3: Important processing parameters and resulting microstructural features for Bimodal microstructures

<table>
<thead>
<tr>
<th>Step</th>
<th>Important parameters</th>
<th>Microstructural Features</th>
</tr>
</thead>
<tbody>
<tr>
<td>Homogenization in the $\beta$ phase field</td>
<td>Cooling Rate</td>
<td>GB $\alpha$ layer</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Width of $\alpha$ lamellae ($\alpha_p$ Size)</td>
</tr>
<tr>
<td>Deformation in the $\alpha+\beta$ phase field</td>
<td>Deformation Temperature</td>
<td>Texture Type</td>
</tr>
<tr>
<td></td>
<td>Deformation Degree</td>
<td>Texture Intensity</td>
</tr>
<tr>
<td></td>
<td>Deformation Mode</td>
<td>Dislocation Density</td>
</tr>
<tr>
<td>Recrystallization in the $\alpha+\beta$ phase field</td>
<td>Recrystallization Temp.</td>
<td>$\alpha$ volume %</td>
</tr>
<tr>
<td></td>
<td>Recrystallization Time</td>
<td>($\beta$ grain size)</td>
</tr>
<tr>
<td></td>
<td>Cooling Rate</td>
<td>Alloy element partitioning</td>
</tr>
<tr>
<td>Aging at $\alpha+\beta$ phase field</td>
<td>Aging temperature</td>
<td>$\text{Ti}_3\text{Al}$ in $\alpha$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Secondary $\alpha$ in $\beta$</td>
</tr>
</tbody>
</table>

Table 2.4: Influence of Microstructural parameters on Mechanical Properties of $\alpha+\beta$ Ti-alloys

<table>
<thead>
<tr>
<th>$\alpha+\beta$ Titanium Alloys</th>
<th>$\sigma_f$</th>
<th>$\epsilon_f$</th>
<th>HCF</th>
<th>Microcracks $\Delta K_{th}$ $R=0.7$</th>
<th>Macrocracks $K_I$ $R=0.1$</th>
<th>Creep Strength $0.2%$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aging ($\alpha_1$) Oxygen</td>
<td>+</td>
<td>-</td>
<td>+</td>
<td>-</td>
<td>-</td>
<td>+</td>
</tr>
<tr>
<td>Bi-Modal Structure</td>
<td>+</td>
<td>+</td>
<td>-</td>
<td>$</td>
<td>$</td>
<td>-</td>
</tr>
<tr>
<td>GB $\alpha$-Layers</td>
<td>0</td>
<td>-</td>
<td>-</td>
<td>$O$</td>
<td>-</td>
<td>$O$</td>
</tr>
<tr>
<td>Small $\alpha$-Colonies</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$\alpha$-Lamellae</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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Figure 2.1: Schematic phase stability fields in Ti alloys of various compositions

Figure 2.2: Schematic diagram of β processing heat treatment
Figure 2.3: Schematic CCT diagram showing the effect of cooling rate on the constitution of an $\alpha + \beta$ Ti alloy after continuous cooling.

Figure 2.4: Light micrographs showing the difference in morphology and scale of (a) the martensitic transformation product (b) and the nucleation and growth product in Ti-6Al-4V quenched and air cooled, respectively, from above the $\beta$ transus.
Figure 2.5: Prior β grain boundary decorated by α phase

Figure 2.6: Schematic CCT diagram similar to that one in fig. 1 but also showing the dashed C curve for grain boundary α formation
Figure 2.7: Schematic diagram showing $\alpha/\beta$ processing steps

Figure 2.8: (a) The penetration of $\beta$ phase into the $\alpha/\alpha$ boundaries is determined by an interfacial energy balance. The smaller the dihedral angle $\theta$, the deeper is the penetration (b) An example of penetration of $\alpha$ by $\beta$ at such a boundary
Figure 2.9: Schematic illustration of the formation of a Widmanstätten structure in a Ti-6Al-4V alloy by cooling slowly from above the β transus.
Fig 2.10:  a) lamellar microstructure (Optical micrograph: bright phase is $\alpha$ phase)  
   b) bimodal microstructure (SEM micrograph: dark phase is $\alpha$ phase)
Figure 2.11: a) Y.S and b) tensile ductility as a function of cooling rate; closed symbols: large $\beta$ grain size, open symbols: small $\beta$ grain size
Fig 2.12: Tensile property variation with amount of primary $\alpha$ in a) Hylite 50 and b) IMI 679 alloys
CHAPTER 3

MICROSTRUCTURE EVOLUTION IN \(\alpha/\beta\) Ti ALLOYS-
DEVELOPMENT OF COLONY & BASKEWEAVE MICROSTRUCTURES

3.1 Introduction:

When heat-treated in the \(\beta\) phase field, \(\alpha/\beta\) titanium alloys develop the Widmanstätten microstructure. Typically, if the cooling rate following the heat treatment is relatively slow, a colony microstructure, consisting of groups of \(\alpha\) laths belonging to the same crystallographic variant (colony), develops. In contrast, when employing faster cooling rates, a basketweave microstructure develops. The basketweave microstructure consists of multiple variants of \(\alpha\) laths clustered in the same region. This chapter addresses microstructural evolution in \(\beta\)-annealed \(\alpha/\beta\) Ti alloys with an emphasis on the factors influencing the formation of the colony and basketweave microstructures.

It is well known that the laths of the hcp \(\alpha\) phase generally exhibit a Burgers orientation relationship (OR) with the matrix bcc \(\beta\) phase in these Ti alloys. The Burgers OR is \((0001)_{\alpha}||\{110\}_{\beta}\) and \(<1\overline{1}20>_{\alpha}||<1\overline{1}1>_\beta\) [69]. The same OR is also observed between the grain boundary (GB) \(\alpha\) precipitates and the \(\beta\) matrix [70, 71]. It is typically not possible for the GB \(\alpha\) to form while maintaining the Burgers OR with both the
adjacent β grains. Thus, the GB α maintains the Burgers OR with the β phase in one of the adjacent grains, and it generally chooses a specific orientation that allows it to have as small a deviation from the Burgers OR as possible with the other grain [70]. As a result, it is also able to maintain partial coherency with the β grain on the “non-Burgers” side, because the interface will have ledges and misfit-compensating dislocations [72]. It has also been reported that the variant of α selected at the prior β grain boundary is the one which allows a very small angle between the matching $<\overline{1120}>_\alpha||<111>_{\beta}$ direction and the grain boundary plane [70]. While these detailed studies in the published literature [70-72] have addressed the OR between the GB α precipitates and adjacent β grains as well as the structure of the α/β interface, the subsequent development of the microstructure within the grains of the β matrix and the influence of the GB α precipitates on this microstructural evolution has not been critically addressed. In particular, there is very little known regarding the details of the formation of the colony and basketweave microstructures, despite the recognition that such microstructural details play a dominant role in determining the mechanical properties of these alloys. While the previous work, reported in the published literature, has investigated the formation of side-plates of α from the GB α precipitates [70,73], the selection of α variants and further growth of these side-plates during the solid-state transformation resulting in the contrast between the final microstructures (colony versus basketweave) has not been investigated in detail.

In the present research, a series of step-quenching and isothermal holding experiments have been carried out to capture the microstructure at different stages of its development. Details of these experiments and their results will be discussed here. In the
following sections, the factors affecting the colony/ basketweave microstructure formation will be discussed following which a model will be proposed for basketweave microstructure development.

3.2 Experimental Details- Colony/ Basketweave formation:

3.2.1 Selection of Material: To study the microstructure evolution in \(\alpha/\beta\) Ti alloy, the first task was to select the alloy on which this study can be effectively carried out. This microstructure evolution study should be done on a Ti alloy which shows similar morphology of the microstructure as the most commonly used \(\alpha/\beta\) Ti alloy, Ti-6Al-4V. However, Ti-6Al-4V alloy for this study was unfavorable because a few early experiments showed that arresting the microstructure evolution at different stages of its development is extremely difficult in this alloy because both alloying elements (Al and V) have relatively large diffusivity. Thus, in Ti-6Al-4V, once the laths start to grow, they grow very fast to reach the final stable microstructure at the corresponding temperature. Formation of large amount of \(\alpha'\) martensite is also another problem faced with alloy containing such a low volume fraction of \(\beta\) stabilizer as does Ti-6Al-4V.

Based on some early experiments with other commercially available alloys (Ti6246, Ti62222, Ti550), as well as a laboratory processed model alloy (Ti-3Al-10V) it was decided the best candidate for the microstructural evolution study is the alloy Ti550 (Ti - 4%Al - 4%Mo – 2%Sn - 0.5%Si). The microstructure of Ti550 is similar to that of Ti-6Al-4V, but it has Mo as a \(\beta\) stabilizing element, which is a much slower diffusing
element than V, resulting in a slower growth of the $\alpha$ laths during isothermal holding at sub-transus temperature. The result is that the arrest of microstructure at successive stages easier. Also, the presence of Mo (an effectively stronger $\beta$ stabilizer) decreases the chance of formation of martensite in this alloy during quenching.

So, for the present research, Timetal 550 (Ti - 4%Al - 4%Mo - 2%Sn - 0.5%Si) supplied by Timet Company has been used as a candidate $\alpha/\beta$ alloy. The material was received in an isothermally forged condition, which was then sectioned into 1cm$^3$ pieces.

3.2.2 Heat Treatments:

3.2.2.1 Undercooling effect on Microstructure evolution:

The $\beta$ transus temperature of this alloy is approximately 975°C. Therefore, the samples were solutionized 60°C above $\beta$ transus at 1035°C, and held there for 45 minutes. Then, the samples were step quenched to different temperatures below the $\beta$ transus, at 900°C, 800°C, 700°C and 600°C, and were held at each temperature for 2 minutes, 5 minutes and 10 minutes, and subsequently quenched in water in order to arrest the microstructural evolution. The schematic of these heat-treatment schedules is shown in figure 3.1.

3.2.2.2 Prior $\beta$ grain size effect on Microstructure evolution:

In order to produce different prior $\beta$ grain sizes, samples were heated above the $\beta$ transus, at 1100°C, for different times. One sample was
solutionized at 1100°C for 15 minutes, while the other was solutionized for 4 hours. Samples were then step quenched to 700°C and were held at that temperature for 5 mins before they were water quenched. Schematics of these heat-treatments are shown in figure 3.2.

The heat treatments were performed using two horizontal tube furnaces kept side by side. The picture of the arrangement is shown in figure 3.3. One furnace was kept at a temperature above β transus, (1035°C or 1100°C), while the other was kept at a sub-transus temperature (900°C, 800°C, 700°C or 600°C). After solutionizing in the first furnace, the sample was pushed to the center of the next tube furnace very quickly to simulate the step quench experiment from 1035°C to one of the selected sub-transus temperature. After holding the sample at the sub-transus temperature for a selected time, it was pushed out of the tube furnace into a container with cold water for quenching.

The environment was not controlled in this experimental arrangement, but to decrease oxidation on the surface of the samples, each sample had been wrapped with titanium foil. For easy transport of the sample, each wrapped sample was placed in a small ceramic boat, which was pushed by a rod to move the sample from one furnace to another and also to push it out of the furnace during quenching.

3.2.3 Metallography and Characterization: The samples were sectioned along the center after heat-treatment, and the cut surfaces were polished initially by SiC abrasive papers down to 6 µm level and then using colloidal silica to 0.05 µm level. Centers of the cut surfaces were imaged using the FEI Sirion SEM using a backscatter
electron detection mode. Cutting the sample and imaging the center part were done to ensure that any oxygen effect at the surface was not being analyzed. In addition, the crystallography of the α and β phases was studied using orientation imaging microscopy carried out in a FEI XL30 SEM equipped with an EBSD detector and using the TSL OIM software.

3.3 Under-Cooling Effect on Microstructure Evolution- Microscopy Results:

In this section, scanning electron micrographs will be shown for differently heat-treated samples. All samples shown here were first solutionized at 1035°C, following which they were step quenched to 4 different sub-transus temperatures, and at each temperature 3 different hold times were carried out to see the time evolution of the microstructure at that temperature. So, a total of 12 heat treatments have been carried out. Figure 3.4 shows microstructures of the 3 samples which were held at 900°C for 2 mins, 5 mins and 10 mins respectively. The sample held for 2 mins shows that α phase has precipitated on the grain boundaries and colonies of α laths started to grow from the grain boundary α. Images of the samples held for 5 mins and 10 mins show a progressively increased volume fraction of α phase in the microstructure. More colonies of α laths grow from grain boundary α as the sample is held for a longer time. An interesting point to note here is that, even when held for 10 minutes at 900°C, the microstructure has not transformed fully. This is because of the very low equilibrium volume fraction of α at that high temperature. The sample held for 10 mins shows some intragranular colonies of α laths, but they might be due to the sectioning effect; in other words, they may have
nucleated from some grain boundary $\alpha$ below or above the imaged surface. This occurrence of intragranular $\alpha$ phase being seen in a 2d image will be further addressed in subsequent sections.

Figure 3.5 shows the microstructures of the samples which were held at 800$^\circ$C for 2 mins, 5 mins and 10 mins respectively. For the samples held at 2 mins, early stages of the nucleation and growth of the $\alpha$ phase on the prior $\beta$ grain boundaries are visible. Few $\alpha$ side plates have started growing from the grain boundary $\alpha$. Upon holding for 5 mins, different colonies of $\alpha$ laths have grown from the grain boundary $\alpha$ towards the grain interior, progressively growing with time. After 10 mins, almost the entire grain has transformed to the colony microstructure. Interestingly, no basketweave region is formed at 800$^\circ$C (an undercooling of around 175$^\circ$C below the $\beta$ transus).

Holding at 700$^\circ$C will result in a greater under-cooling, and it is seen that different variant colonies of $\alpha$ laths start forming from the grain boundaries. After a certain distance, a few $\alpha$ laths of each colony will continue grow while other laths stop. Those few laths from different colonies which shoot inside the grain give the appearance of a cluster of different variants at the center of the grain (See figure 3.6a)), leading to the development of a basketweave type of microstructure. Figure 3.6b) and 3.6c) show the microstructure of samples which were held at 700$^\circ$C for 5 mins and 10 mins respectively. The equilibrium volume fraction of $\alpha$ phase is much higher compared to the samples held at higher as temperature. Samples held at this temperature show a mixed mode of microstructure containing both colony and basketweave regions. It is interesting to note that isothermal holding is giving rise to basketweave microstructure formation by the
extension of $\alpha$ laths from different variants of colonies growing from the grain boundary $\alpha$, which is in contrast to a commonly speculated belief that basketweave forms during continuous cooling at lower temperatures by homogeneous nucleation and growth of different variants of $\alpha$ laths.

Figure 3.7 shows the microstructures of the samples held at $600^0C$ for 2 mins, 5 mins and 10 mins. The microstructure is predominantly basketweave type throughout the grain interior. A small volume fraction of colonies near the grain boundaries is also visible (figure 3.7 (a) and (b)). It should be noted that, compared with the samples held at $700^0C$, much thinner layers of colonies have formed case.

Interesting observations from the above discussion can be summarized in few points. For the study of microstructure evolution with time and temperature variation in $\alpha/\beta$ Ti alloys, step-quenching and isothermal holding experiments have been performed. It has been seen that formation of basketweave microstructure is a function of undercooling. At higher temperature and lower undercooling, mostly colonies of $\alpha$ laths form. The tendency of the formation of basketweave microstructure increases with increasing undercooling, causing an increase in the volume fraction of basketweave with increasing undercooling. Thickness of colonies near the grain boundaries decreases with increasing undercooling. In addition, it appears that the basketweave microstructure might be forming by extension of a few laths from different colonies inside the grain; this will be further discussed in detail in the following sections. In order to study this issue in further detail the influence of prior $\beta$ grain size on microstructure evolution at a constant under-cooling has been investigated.
3.4 Prior β grain size effect on Colony/ Basketweave formation- Microscopy Results:

In order to compare the influence of different prior β grain sizes on the microstructural evolution two samples with distinctly different grain size were step quenched to 700°C, such that they experience identical undercooling.

As can be seen from 3.8, while the samples held for 15 mins above the β transus shows grain sizes ranging from 100 µm to 300 µm, the other sample, which was held at the same temperature for 4 hours, shows grains of size 600 µm or bigger. A few interesting observations, which to lead to some kind of model for basketweave microstructure formation, will be discussed in the next few paragraphs.

In the case of small grains of size 100 – 200 µm, the entire grain is typically consists of colonies of α laths, showing no basketweave region as shown in figure 3.9. On the other hand, grains of size larger than 200 µm show a mixed microstructure with colonies near grain boundaries and basketweave at the grain interior. Examples are shown in figure 3.10a) through 3.10c).

The next interesting observation was that when a colony grows from grain boundary α, until a characteristic length of 80 –100 µm, all α laths in that colony appear to grow together; then fewer laths continue grow inside while others stop, as if a few laths are shooting inside the grain from each colony. This characteristic length, through which α laths in a colony grow together, appears to be independent of the prior β grain size. This will be evident from figures 3.11 and 3.12. Figure 3.11 shows examples of small or intermediate size grains where the characteristic length for different colonies
through which all $\alpha$ laths in the colony grow together, is around 80 - 100 $\mu$m. This characteristic length remains constant even in large grains too, examples of which are shown in figure 3.12.

It is also interesting to note that, while a colony grows from grain boundary $\alpha$, beyond the characteristic length of 80 –100 $\mu$m mentioned above (first zone), progressively fewer laths continue grow inside and others stop (second zone). If the colonies are allowed to grow further, even fewer laths will continue growing inside, giving a “single laths shooting inside” type appearance (third zone). This phenomenon is shown in figures 3.13 and 3.14 for the case of intermediate or large prior $\beta$ grains, where colonies growing from grain boundary $\alpha$ show three distinct zones. The consequence of this may be seen in the difference in appearance of the basketweave region in very large grains and in smaller (intermediate size) grains. In very large grains, basketweave region appears to consist of single laths (needle like appearance) of different variants. In the case of smaller grains, the basketweave region at the center of the grains appears to consist of different variants, each containing a bunch of $\alpha$ laths. A comparative picture of the basketweave region at the center of the grain as a function of grain size is shown in figure 3.15.

Also, when the prior $\beta$ grain size is small, of the order of less than twice of that characteristic length mentioned here, the entire grain exhibits a colony microstructure. This has been discussed in figure 3.9.
3.5 Variant Selection during microstructure evolution - Colony/ Basketweave formation

When a second phase is precipitated in the parent matrix phase (in this case \( \alpha \) phase in \( \beta \) matrix), the product phase tries to maintain coherency as much as possible with the parent phase to reduce the activation energy of nucleation; in the process, a specific rational orientation relationship is maintained between the two phases [71]. When the crystal structures of the two phases are different, for a given orientation relationship, there are several equivalent orientations of the product phase, which are called variants [71]. In the case of hcp \( \alpha \) formation in the bcc \( \beta \) matrix, a Burgers OR (\( \{0001\}_\alpha \parallel \{110\}_\beta \) and \( <1120>_{\alpha} \parallel <1\bar{1}1>_{\beta} \)) is often maintained. There are three close packed \( <11\bar{2}0>_{\alpha} \) directions on the \( (0001)_\alpha \) plane and two close packed \( <111>_{\beta} \) directions on the \( (110)_\beta \) plane. Thus, there are six possible combinations of parallel close packed directions between \( \alpha \) and \( \beta \) phases. Due to the presence of 6\( _3 \) symmetry along \( [0001]_\alpha \), the three \( <11\bar{2}0> \) directions are equivalent. So, among the six combinations only two combinations of parallel directions on any one \( \{110\}_\beta \) plane are distinguishable. As there are six possible \( \{110\}_\beta \) planes in the bcc \( \beta \), there are 12 variants of the Burgers OR. When \( \alpha \) laths nucleate and grow from the GB \( \alpha \) at the prior \( \beta \) grain boundary to form either a colony or a basketweave microstructure, one or multiple specific variants (among the possible 12) are selected according to certain crystallographic criteria.
A previous study [74] showed that typically, for a random grain boundary, the GB \( \alpha \) exhibits a Burgers OR with only one of the adjacent prior \( \beta \) grains, and colonies nucleate and grow from the GB \( \alpha \) into that \( \beta \) grain with which it exhibits the Burgers OR. This can be seen in Figure 3.16 [74].

On the other side of the grain boundary, where the basketweave microstructure starts forming near the grain boundary, a number of clusters of \( \alpha \) laths belonging to different variants have been identified. The \( \alpha \) laths in the clusters maintain Burgers OR with the \( \beta \) matrix in the corresponding grain. From this OIM study of such clusters of \( \alpha \) laths in the basketweave region, it is seen that \( \alpha \) laths in any cluster select their variants according to some particular crystallographic criteria. From pole figures shown in Figure 3.17 [74], it appears that the \( \alpha \) laths in the cluster comprising the basketweave microstructure either share a common \([11\bar{2}0]\), which is parallel to the Burgers \([111]\) of the \( \beta \) grain, or share a common \((0001)\), which is parallel to the Burgers \((011)\) of \( \beta \). Based on the study of different clusters of \( \alpha \) laths, these two possible variant selection criteria have been identified for the formation of the basketweave microstructure. Also, where one set of \( \alpha \) laths seems to nucleate from another variant of \( \alpha \) laths, they select either of the two variants mentioned above. Figure 3.18 shows one such area, where a high resolution OIM scan has been carried out. From the pole figure analysis it is seen that the two variant \( \alpha \) laths share a common \(<1\bar{1}20>\), which is parallel to Burgers \(<111>\) of \( \beta \). Figure 3.19 shows that both the \( \alpha \) variants maintain Burgers orientation relationship with the \( \beta \) phase of the grain.
The clustering of multiple variants of \( \alpha \) laths resulting in the formation of the basketweave microstructure is likely to be influenced by strain energy criteria. Since the solid-state \( \beta \rightarrow \beta + \alpha \) transformation in titanium results in a substantial volume and shape change, the nucleation and growth of \( \alpha \) laths will lead to significant straining of the surrounding \( \beta \) matrix. Therefore, the system will favor the reduction of the overall strain energy via possibly the principle of self-accommodation [75, 76, 77]. The principle of self-accommodation is motivated by the tendency to minimize the total transformation shape strain and the corresponding strain energy by grouping (or clustering) of specific crystallographic variants. Such self-accommodating morphologies have been reported in a number of different martensitic microstructures, such as a triangular grouping of three variants in Zr-2.5\%Nb [76], as well as NiTi-based shape memory alloys [77]. The self-accommodating morphology of martensitic \( \alpha' \) laths forming in quenched pure titanium has been recently discussed by Wang et. al. [78]. In their paper, the shape strain due to each of the 12 variants forming from the martensitic \( \beta \rightarrow \alpha' \) transformation has been calculated as well as the average shape strain resulting from a cluster of three or variants in different combinations. There are six possible types of high-angle grain boundaries possible between the 12 different \( \alpha' \) variants. Their analysis indicates that the greatest degree of self-accommodation of the shape strains occurs when three variants of \( \alpha' \) in two types of clusters are formed. The first type of these clusters consists of three variants of \( \alpha' \) forming high-angle grain boundaries of the type \([1\overline{1}20] / 60^\circ\). For this type of cluster, the three \( \alpha' \) variants would be related by a common \([1\overline{1}20]\) and their basal (0001) planes.
would be rotated by 60°. The second type of cluster that would lead to a high degree of self-accommodation is when the $\alpha'$ variants formed high-angle grain boundaries of the type $[\overline{1}05\bar{5}3] / 63.26^\circ$ [78]. In this case, the $\alpha'$ variants would share a common $[\overline{1}05\bar{5}3]$ axis and be rotated by 63.26° about this axis. Another possible boundary discussed by Wang et. al. [78] is of the type [0001] / 10.53° that would correspond to the $\alpha'$ variants sharing a common [0001] axis (common basal plane) parallel to a specific Burgers <011> pole of the $\beta$ grain and their respective Burgers [1120] axes aligned with the two possible <111> axes lying on the same Burgers (011) plane.

3.6 Proposed Model for Basketweave Microstructure Formation:

Based on the above evidences and discussions a model for basketweave microstructure is proposed here. Various possible nucleation mechanisms for the cluster of variants to form a basketweave microstructure will be addressed in the following sections, and a mostly observed mechanism for the formation of basketweave will be proposed.

3.6.1 Homogeneous Intragranular Nucleation:

Based on the previously-stated results it appears that the commonly held belief regarding the formation of basketweave microstructure by homogeneous intragranular nucleation at lower temperatures during continuous cooling does not appear to be the case. Strictly no direct evidence of such homogeneous nucleation of $\alpha$ variants has been observed.
3.6.2 Heterogeneous Nucleation:

3.6.2.1 Heterogeneity inside the grains:

A cluster of variants of $\alpha$ laths can be formed on some sub-micron size defects present inside the grains. Similar experiments, as mentioned earlier, of step-quenching followed by isothermal holding at sub-transus temperature have been carried out in a laboratory processed model alloy Ti-3Al-10V which shows a similar microstructural morphology to Ti-6Al-4V or Ti-550 alloy. Formation of clusters of variants inside the grain was observed (see figure 3.20a)). At higher magnification in Scanning Electron Microscope (SEM), a darker feature was observed at the center of each star-like cluster of $\alpha$ variants (See figure 3.20b)). To ascertain the nature of this darker feature, a site-specific TEM foil was cut at the center of the $\alpha$ clusters (See figure 3.21) using Focused Ion Beam (FIB). Figure 3.22 shows the bright field image of that TEM foil, which shows that the darker feature at the center of the cluster of $\alpha$ variants is actually a sub-micron size pore inside the grain. Theses sub-micron size pores might have been introduced to the microstructure during the solidification after arc-melting in the laboratory. However, the presence of this type of heterogeneity is not common in the commercially available alloys.

3.6.2.2 Grain Boundary Nucleation of variants:

As mentioned in earlier sections based on the results of present research, it is observed that the primary mechanism for the formation of basketweave is by the shooting
of a few $\alpha$ laths into the grain interior from different colonies growing from the grain boundary $\alpha$. These laths intersect and give the basketweave appearance (See figure 3.23). When a colony grows from grain boundary $\alpha$, beyond a characteristic length, progressively fewer laths continue grow inside and others stop. If the colonies are allowed to grow further, even fewer numbers of laths continue growing inside, giving a “single laths shooting inside” appearance. This happens from different variant colonies, resulting in a basketweave region at the center of the grains. The reason for this progression is that the growth of other laths is stopped because laths of other variants from neighboring colonies start intersecting and stop some of the laths of the initial colony from growing. That is how some laths in the same colony grow longer while others are truncated by intersecting laths from a different colony.

Sometimes, a few $\alpha$ laths observed inside the grain don’t show any connection with the grain boundary $\alpha$ on the surface view. To understand where those $\alpha$ laths nucleate from, Focused Ion Beam was used to cut trenches at different positions. One such example is shown in figure 3.24. It is seen from figure 3.24c) that the laths have connections with the grain boundary $\alpha$ below the viewing surface, which is evident from the perpendicular surface of the trench. So, inside grain $\alpha$ laths might actually have connections with the grain boundary $\alpha$ below the surface; they actually nucleate from the grain boundary $\alpha$ below the surface.
3.6.2.3  Nucleation of variant from an already grown variant of $\alpha$ laths:

The mechanism stated in the previous section has been proposed as the primary mechanism to form basketweave, some inside grain heterogeneous nucleation from the side of another $\alpha$ variant is also observed as described in figure 3.18. OIM results (Figure 3.19) of this region shown previously reveal that the second variant of $\alpha$ laths share a common 1120 with the $\alpha$ variant from which it appears to nucleate. This sharing of particular variant suggests that one of the variants has been nucleated from the other. To be further investigate this nucleation phenomenon, a site-specific TEM foil was cut from the intersection of these two variants using FIB; a thin $\beta$ layer has been observed between the two variants of $\alpha$ laths. The presence of an $\alpha/\alpha$ boundary would have been strong evidence of nucleation of the second variant from the first variant; however it is possible that this presence of thin layer of $\beta$ might be due to the sectioning effect.

It is proposed that basketweave microstructure is formed primarily by the shooting of a few laths inside the grain interior from different colonies growing from grain boundary $\alpha$. Upon further under-cooling, new variants of $\alpha$ laths might nucleate from the already grown $\alpha$ laths.
Figure 3.1 Isothermal Holding Experiments to study the under-cooling effect on microstructure evolution
Figure 3.2 Isothermal Holding Experiments to study the prior β grain size effect on microstructure evolution

Figure 3.3: Experimental Arrangement for Step-Quenching experiments
Figure 3.4 Microstructure of Ti550 sample when heat treated as follows: a) $1035^\circ C$ for 45 mins, step quenched to $900^\circ C$, held there for 2 mins, then water quench (WQ). b) $1035^\circ C$ for 45 mins, step quenched to $900^\circ C$, held there for 5 mins, then water quench (WQ). c) $1035^\circ C$ for 45 mins, step quenched to $900^\circ C$, held there for 10 mins, then water quench (WQ).
Figure 3.5 Microstructure of Ti550 sample when heat treated as follows: a) $1035^\circ$C for 45 mins, step quenched to $800^\circ$C, held there for 2 mins, then water quench (WQ). b) $1035^\circ$C for 45 mins, step quenched to $800^\circ$C, held there for 5 mins, then water quench (WQ). c) $1035^\circ$C for 45 mins, step quenched to $800^\circ$C, held there for 10 mins, then water quench (WQ).
Figure 3.6 Microstructure of Ti550 sample when heat treated as follows: a) $1035^\circ$C for 45 mins, step quenched to $700^\circ$C, held there for 2 mins, then water quench (WQ). b) $1035^\circ$C for 45 mins, step quenched to $700^\circ$C, held there for 5 mins, then water quench (WQ). c) $1035^\circ$C for 45 mins, step quenched to $700^\circ$C, held there for 10 mins, then water quench (WQ).
Figure 3.7 Microstructure of Ti550 sample when heat treated as follows: a) 1035°C for 45 mins, step quenched to 600°C, held there for 2 mins, then water quench (WQ). b) 1035°C for 45 mins, step quenched to 600°C, held there for 5 mins, then water quench (WQ). c) 1035°C for 45 mins, step quenched to 600°C, held there for 10 mins, then water quench (WQ).
Figure 3.8 a) Small Prior $\beta$ grain size; sample held above $\beta$ transus for 15 mins b) Large prior $\beta$ grain size, sample held above $\beta$ transus for 4 hours.
Figure 3.9: Small grains (of size 100 µm – 200 µm) consist of 100% colony inside the grains.
Figure 3.10: Large grains consist of colonies near grain boundaries; basketweave at the grain interior.
Figure 3.11: Characteristic Length through which $\alpha$ laths in a colony grow together before fewer laths stop growing, is independent of grain size. Here these 3 micrographs are examples of small or intermediate size prior $\beta$ grains.
Figure 3.12: Characteristic Length through which $\alpha$ laths in a colony grow together before fewer laths stop growing, is independent of grain size. Here these 3 micrographs are examples of large prior $\beta$ grains.
Figure 3.13: Three distinct zones of colony; different examples

Example 1
- Even fewer laths continue growing: “Single laths shooting inside” type appearance

Example 2
- Even fewer laths continue growing: “Single laths shooting inside” type appearance

α laths growing together in a colony
Example 3

α laths growing together in a colony

Even fewer laths continue growing: “Single laths shooting inside”

Fewer α laths continue growing

Even fewer laths continue growing: “Single laths shooting inside”

Figure 3.14: Three distinct zones of colony growing from grain boundary to the interior of the grain.
Figure 3.15: Comparative study of basketweave region morphology between intermediate and large prior β grains
Figure 3.16 [74]: Colony grows in that side of the grain, $\beta$ of which has the Burgers orientation relationship with the grain boundary $\alpha$. 
Figure 3.17 [74]: OIM Study of cluster of α laths. While lath 1 and lath 2 share common 0001; lath 2 and lath 3 in the cluster share a common 1120.
Figure 3.18: Horizontal laths nucleating from inclined laths; both variants share a common 1120
Figure 3.19: variant a) and variant b) maintain Burgers OR with the $\beta$ in the grain
Figure 3.20: SEM image of microstructure of Ti-3Al-10V showing inside grain star-like cluster of variants

Figure 3.21: A site specific TEM foil was prepare using FIB along the line shown.
Figure 3.22 Bright field image of the cluster of variants. Variants nucleating from a sub-micron size pore inside the material.

Figure 3.23: Primary mechanism of basketweave microstructure formation by shooting of few laths from different variant colonies.
Figure 3.24: α laths connected with grain boundary α below the viewing surface.
CHAPTER 4

MICROSTRUCTURE CHARACTERIZATION AND DATABASE DEVELOPMENT

In order to develop a microstructure-based database for the purpose of training a Neural Network, the important microstructural features must first be identified and subsequently quantified.

4.1. Identification of Microstructural Features to Characterize: As mentioned in the literature review section, researchers have identified several microstructural features that significantly impact the deformation mechanisms and consequently the mechanical properties of both $\beta$-processed and $\alpha+\beta$-processed $\alpha/\beta$ titanium alloys. According to Lutjering et.al.[79], the critical microstructural parameters for fully lamellar structures with respect to mechanical properties are the $\beta$ grain size, the colony size, the width of the $\alpha$ lamellae, and the character of the inter-lamellar interface. They cited the grain boundary $\alpha$, which may be considered as a continuous thin layer along prior $\beta$ grain boundaries, as another factor which might influence mechanical properties. Properties exhibited by samples with both large and small prior $\beta$ grain sizes were compared. It was
discovered that, while prior β grain size has little or no influence on yield strength, it has a strong influence on ductility. Boyer and Wallem [80] attempted to correlate the microstructural features of β-annealed Ti-6Al-4V of each condition with tensile strength and ductility. However, it was not possible to establish a correlation between the mechanical properties and prior β grain size, colony size or α plate width. It was suggested that the tensile property-microstructure relationship must be determined by a complex combination of individual parameters. Rhodes. et.al.[81] made a similar observation when attempting to establish a correlation of microstructural features to fatigue crack growth rate. Ambard et. al.’s [82] work on the deformation mechanism of Ti-6Al-4V indicates that a colony behaves as a single grain within which only the basal system is activated, while in a globular grain many glide systems can be activated. It was argued that this is the reason for the α colonies being more detrimental to ductility than the globular grains. Thus, during colony deformation, many dislocations of the same nature pile up at the colony boundaries and produce a high stress concentration. As a consequence, damage is expected to nucleate at colony boundaries. These authors suggested that the colony size is an important microstructural parameter as far as ductility is concerned. According to researchers [83, 84], the thickness and aspect ratios of α laths impact ductility, fatigue crack initiation, strength, and creep mechanisms. Interfaces between α and β phases impact the slip between α laths and between prior β grain boundaries [85].
Phase Field models and diffusion-based mechanistic models have recently been
developed to predict grain growth and grain-boundary $\alpha$ thickening. Validation of these
models require extensive characterization of experimental data with model predictions.

Based on the current understanding of deformation behavior in $\alpha/\beta$ Ti alloys such
as Ti-6Al-4V described above, the microstructural features that have been identified for
quantification are as follows.

For $\beta$-processed $\alpha/\beta$ Ti alloy:

1. thickness of Widmanstätten $\alpha$-laths
2. Colony Size
3. Prior $\beta$ grain size
4. Volume fraction of $\alpha$
5. Volume fraction of Basketweave microstructure
6. Width of grain boundary $\alpha$
7. Mean edge length of $\alpha$-laths
8. Tortuosity of the colony boundary
9. Fraction of prior $\beta$ grain boundary occupied by $\alpha$

For $\alpha+\beta$ processed Ti alloy:

1. Volume fraction of globular $\alpha$
2. Thickness of $\alpha$ laths in transformed $\beta$ region
3. Mean globular $\alpha$ grain size.
4.2 **Sources of samples used for database building:** The samples used to construct the database came from different sources, as will be explained in detail in this section.

4.2.1 **For Tensile Property of $\beta$ heat-treated samples:** The samples for the tensile property database came from two separate sources. The first set of samples was laboratory processed, and the second set of samples was obtained from industry through the Materials Affordability Initiative (MAI) program. Two separate databases have been developed, one containing the laboratory-processed samples and the other containing the industry provided samples. In order to rapidly heat-treat the samples to produce a wide range of microstructures, a novel approach was taken. A Gleeble™ 1500 thermomechanical simulator was used for carrying out the heat treatments on Ti-6Al-4V. A total of 72 samples were heated to a temperature of $1050^\circ$C (above the $\beta$-transus of Ti-6Al-4V), where the samples were held for either 1 or 5 seconds and then cooled using one of two different cooling rates ($16.7\,^\circ$C/s or $2.78\,^\circ$C/s) to a temperature of $300^\circ$C. The samples were aged to a temperature below the $\beta$-transus ($670-970\,^\circ$C) for 300 seconds and cooled down at either of the three different cooling rates ($16.7, 2.78$ or $0.278\,^\circ$C/s). A total of 86 more $\beta$-processed samples were obtained from industry partners, which made up the second database for tensile property modeling for $\beta$-processed Ti-6Al-4V. Samples have been undergone three different broad categories of thermomechanical treatments that are schematically shown in figure 4.1. It was recognized and suggested in one of the MAI meeting that samples which had undergone thermo-mechanical schedule
1 (in figure 4.1) should be termed as β-processed samples, and should be separated out from the rest of the samples in the database. The rest of the samples, which were subjected to thermo-mechanical schedules 2 and 3, are termed β-annealed samples because in the final step of the treatment they were taken above β-transus temperature whereby their previous mechanical treatment history was lost. It was also mentioned that for Ti-6Al-4V, β-anneal treatment is the more typical industrial practice. So, 52 β-annealed samples were separated out to remodel the tensile properties.

A wide range of microstructures were obtained by the following β anneal treatments. Samples were forged at either 968°C or 1032°C to strains of either 40% or 80%; post forging they were re-heated to a temperature of 1032°C to solutionize above β transus. Following this step, they were cooled down at either of the following three cooling rates: 0.37°C/sec, 1.85°C/sec or 3.7°C/sec. Samples were then aged at either 593°C, 649°C or 704°C for either 2hrs, 4hrs or 8 hrs.

The β-processed samples were forged above the β transus at 1032°C. Post-forging, they were solutionized below β transus temperatures. As a result, the high temperature deformed structure was not fully erased; showing a more deformed grain boundary structure in the β processed samples. Figure 4.2 compares the β annealed and β processed microstructures.

4.2.2 For Tensile Properties of α+β heat-treated samples: 34 α+β heat-treated samples were obtained as baseline samples through the MAI program. To obtain a
wide range of bimodal microstructures, samples were forged in the $\alpha+\beta$ region at 968$^0$ C
to strains of 40% and 80%; they were then solutionized below the $\beta$ transus at 970-980$^0$
C, from which they were cooled at either of the following three cooling rates 0.37
$^0$C/min, 1.85 $^0$C/min or 3.7 $^0$C/min. The samples were then aged at either of 593$^0$ C, 649$^0$
C or 704$^0$ C for either of 2hrs, 4 hrs or 8 hrs.

4.2.3 For Fracture Toughness Database: 86 $\beta$ heat-treated (which includes 52
$\beta$ annealed and 34 $\beta$ processed) samples and 34 $\alpha+\beta$ heat treated Ti-6Al4V samples were
obtained through the MAI program. TiMet provided the ingots, Ladish Company forged
the ingots, and GE heat-treated the samples. Similar heat treatment schedules as those for
the tensile property samples were applied to obtain the variety of microstructures in this
database.

4.3 Metallography of the samples: The samples were metallographically
polished to 0.05 µm using colloidal silica and then imaged using scanning electron
microscopy in a FEI Sirion SEM operating in the backscattered electron imaging mode.
The samples were also etched with Kroll’s etchant and imaged using optical microscopy
in a Nikon Epiphoto optical microscope using reflected light. Each specimen was imaged
at four random positions, though some operator discretion was introduced to avoid
overlap and edge effects. The Sirion SEM micrographs were imaged using an
accelerating voltage of 15 keV and a spot size of four, which provided resolution on the
order of 2.0 nm. Images were captured using a scan speed of 116.7 ms with a resolution
of 3872 × 2904 pixels operating in 8 bit XHD mode. The resolution of the optical images was 1240 × 940 pixels taken in 8 bit. More recent optical images include 50x and 200x image mosaics put together using a Leica DM-IRM microscope and Clemex Vision Professional software. All images were saved using the uncompressed tagged image file format (tiff).

4.4 Quantification of microstructural features: After the digitized images were acquired, the next step was to quantify the selected microstructural features. Microstructural features were quantified using stereological procedures. Stereology [86] is the science of the geometrical relationships between a structure that exists in three dimensions and the images of that structure that are fundamentally two-dimensional (2D). Using stereology, three dimensional information is obtained from two dimensional images, which in the present case are digitized SEM and optical images.

4.4.1 Stereological Procedures: The grayscale images obtained by SEM were converted to binary images using a thresholding procedure. Using this procedure, shades of gray that exists in both the α and β phases were removed to better delineate the contrast between the features. In thresholded binary images, the β phase was represented as white and the α phase by black. This process sets the stage for quantification of the microstructural features using stereological procedures.

The stereological procedures were performed on personal computers running Adobe Photoshop® 7.0 and a commercial plug-in set known as Fovea Pro® 3.0. These
plug-ins allowed for advanced image control and analysis for 8bit, 16bit and higher images.

4.4.1.1 Thickness of Widmanstätten α laths: To measure the thickness of α laths, a set of random lines is drawn on the image; any portions of lines that are on the β phase keep erased, leaving a set of line segments (of length λ) which were only on the α phase (See fig. 4.3). Evaluating different images of the sample and repeating the above steps provided a table of different line lengths (λ). By inverting the lengths and calculating the mean value, the mean thickness of the laths was calculated from the following relation [87]:

\[
\text{lath thickness} = \left( \frac{1}{1.5} \left( \frac{1}{\lambda} \right)_{\text{mean}} \right)
\]

The factor 1.5 comes from the stereological relationship by which the thickness of infinite α laths can be estimated by the line segments which are the intersections of the lines with those α laths.

4.4.1.2 Colony Size Factor: Colonies are clusters of α laths belonging to the same crystallographic variant. Acknowledging the fact that it is difficult to determine the size of colonies without making assumptions about their shape and morphology [86] and also the fact that three-dimensional imaging of Ti-6Al-4V has shown a very complicated shape which is not easy to characterize or generalize [88], colony size is estimated by a
colony size factor using a mean intercept length method. Conceptually the colony size factor is the average length of a randomly oriented line (in three dimensions) that intersects the colony. Colony size factor has a dimension of length that represents the colony size; it is named as “size factor” as it does not give any information regarding the shape of the colonies. A set of random lines is drawn on the low magnification optical image; all the intersections of those lines with the colony boundaries are marked (See Figure 4.4 [89]). A numerical value for the colony size factor is then obtained by dividing the total line-length by the total number of marks.

4.4.1.3 Prior $\beta$ grain Factor: Like Colonies, prior $\beta$ grains also have complicated shapes, which cannot be easily characterized. So, by stereological methods this feature is measured quantitatively without assuming any shape and is represented by prior $\beta$ grain factor. Prior $\beta$ grain size is indirectly measured by measuring the surface area per unit volume of the grains, which is termed the prior $\beta$ grain factor. On low magnification optical image containing at least 5 or 6 prior $\beta$ grains, a set of cycloids are drawn, and wherever those cycloids intersect the prior $\beta$ grain boundaries are marked (See Figure 4.5 [90]). Prior $\beta$ grain factor is then obtained using the following stereological formula:

$$Prior \beta \ grain \ factor = 2 \times \frac{\text{NumberOfMarks}}{\text{TotalCycloidLength}}$$
It should be noted that the prior $\beta$ grain factor has a dimension of the reciprocal of length; so the larger the value of the prior $\beta$ grain factor, the smaller the prior $\beta$ grain size is.

4.4.1.4 Volume Fraction: In standard stereological procedures, any volume fraction is measured by the number fraction. A regular grid of points is overlaid onto the image, and points that fall onto the feature of interest are marked. Volume fraction of that particular feature is measured by the number fraction of those points, which fall on that particular feature.

For modeling various mechanical properties, we had to measure volume fraction of different features, namely total $\alpha$, basketweave microstructure, globular $\alpha$ (in case of bimodal microstructure). See figures 4.6 and 4.7 [90, 89]. In all cases, the principle for measuring volume fraction previously mentioned is the same.

4.4.1.5 Grain Boundary $\alpha$ Width: The width of the grain boundary decorated by $\alpha$ is measured in a manner similar to that of the Widmanstätten $\alpha$ lath thickness. Random line segments are laid down and kept counted wherever they cross the grain boundary $\alpha$ rather than the $\alpha$ laths. The same equation may be used as for measuring the thickness of the Widmanstätten $\alpha$ laths,

$$GrainBoundary\alpha Width = \left( \frac{1}{1.5 \left( \frac{1}{\bar{\lambda}} \right)_{mean}} \right)$$
where \( \left( \frac{1}{\lambda} \right)_{\text{mean}} \) is the average of the inverse of the line lengths of the segments obtained by the intersection of the grain boundary \( \alpha \) with the line grids.

4.4.1.6 Size of Globular \( \alpha \): In a bimodal microstructure, the mean intercept length measures the size of the globular \( \alpha \). The globules are measured directly by calculating the average size of line length that crosses the grain.

The procedure is now fully automated on thresholded images where globular grains are isolated from the rest of the features to be measured.

4.5 Database Development:

4.5.1 Microstructure Aspect: Different databases have been developed for different mechanical properties of two different broad categories of microstructures: \( \beta \) heat treated colony/basketweave microstructure and \( \alpha+\beta \) heat processed bimodal microstructure.

Based on initial experiments with Fuzzy Logic neural networks, four microstructural features were initially determined to be the most important in terms of influencing the tensile properties in a \( \beta \)-processed colony microstructure of an \( \alpha/\beta \) Ti alloy. These are thickness of \( \alpha \) lath, volume fraction of total \( \alpha \), colony size, and prior \( \beta \) grain size. For fracture toughness modeling, an additional microstructural variable, width of grain boundary \( \alpha \) has been considered important. However, results from Bayesian
neural network modeling introduced another microstructural factor as important, the volume fraction of basketweave microstructure. This feature also has been quantified and added to our most recent database.

For bimodal microstructure, following four microstructural features have been characterized and added in the database: Volume fraction of total \( \alpha \), Volume fraction of globular \( \alpha \), Thickness of \( \alpha \) lath in transformed \( \beta \) region and the mean globular \( \alpha \) grain size.

Our initial tensile property models for \( \beta \)-heat-treated colony/basketweave microstructure were based on two separate databases. The databases contained the values of the thickness of \( \alpha \) lath, volume fraction of total \( \alpha \), colony size factor and prior \( \beta \) grain factor as input parameters and the tensile properties (yield strength, ultimate tensile strength and elongation) as output parameters. Table 4.1 lists the range, average, and standard deviation for the various input and output parameters in the two databases.

In the more recent database for the \( \beta \) annealed samples, the volume fraction of total \( \alpha \) parameter has been taken out and the volume fraction of basketweave microstructure has been included instead. Table 4.2 summarizes the statistics for the values of microstructural parameters for this new database. Similar statistics for other databases are tabulated in table 4.3, 4.4, 4.5.

Some representative micrographs are shown to describe extreme values of the different microstructural features. Figure 4.8 through 4.12 are micrographs showing a comparative study of extreme values of microstructural features for \( \beta \) annealed samples.
Figures 4.13, 4.14 and 4.15 show comparison of extreme microstructural features in $\alpha+\beta$ forged samples.

4.5.2 Mechanical Properties Aspect: All the mechanical testing has been done by Metcut Industries. The mechanical properties for which microstructure based databases have been developed are the tensile properties (yield strength, ultimate tensile strength and % elongation), fracture toughness and creep. For a first approximation of creep modeling of $\alpha+\beta$ forged Ti-6Al-4V samples, stress-strain diagrams have been fitted by the Hollomon equation, $\sigma = K\varepsilon^n \dot{\varepsilon}^m$, and from the parameters of the Hollomon equation, namely $K$ (strength parameter), $n$ (strain coefficient) and $m$ (strain rate coefficient), creep curves have been predicted.

The raw data of different mechanical properties against each individual microstructural variable are plotted (see figures 4.16 through 4.27) to give a clearer picture of range, availability and sparcity of data.
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Minimum Value</th>
<th>Maximum Value</th>
<th>Average Value</th>
<th>Standard Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Colony Thickness of α Lath (µm)</td>
<td></td>
<td>0.14</td>
<td>1.27</td>
<td>0.44</td>
<td>0.23</td>
</tr>
<tr>
<td>Colony Size Factor of Total α</td>
<td></td>
<td>0.86</td>
<td>0.96</td>
<td>0.92</td>
<td>0.02</td>
</tr>
<tr>
<td>Prior β Grain Factor (mm²/m³)</td>
<td></td>
<td>1.1</td>
<td>55.2</td>
<td>7.50</td>
<td>3.48</td>
</tr>
<tr>
<td>Yield Strength (ksi)</td>
<td></td>
<td>103.3</td>
<td>125.8</td>
<td>118.3</td>
<td>4.07</td>
</tr>
<tr>
<td>Ultimate Tensile Strength (ksi)</td>
<td></td>
<td>120.7</td>
<td>145.0</td>
<td>134.1</td>
<td>4.64</td>
</tr>
</tbody>
</table>

Table 4.1: Statistics of the various input and output parameters in earlier databases for β heat treated colony/basketweave microstructure samples
<table>
<thead>
<tr>
<th></th>
<th>VF of Colony</th>
<th>Lath Thickness (µm)</th>
<th>CSF (µm)</th>
<th>GB width (µm)</th>
<th>α PBGF (mm²/mm³)</th>
<th>Toughness (ksi.in¹/²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>min.</td>
<td>0.209</td>
<td>0.157</td>
<td>18.854</td>
<td>0.162</td>
<td>0.812</td>
<td>74.3</td>
</tr>
<tr>
<td>max.</td>
<td>1</td>
<td>0.788</td>
<td>236.412</td>
<td>9.24</td>
<td>3.144</td>
<td>108.4</td>
</tr>
<tr>
<td>average</td>
<td>0.921</td>
<td>0.342</td>
<td>102.734</td>
<td>2.271</td>
<td>2.077</td>
<td>92.1</td>
</tr>
<tr>
<td>standard deviation</td>
<td>0.160</td>
<td>0.170</td>
<td>52.827</td>
<td>1.661</td>
<td>0.571</td>
<td>6.7</td>
</tr>
</tbody>
</table>

Table 4.3: Statistics of the various input and output parameters in the toughness database for β annealed samples

<table>
<thead>
<tr>
<th></th>
<th>VF of Total α</th>
<th>Globular Grain Size (µm)</th>
<th>VF of Globular α</th>
<th>α Thickness in Transformed β (µm)</th>
<th>U.T.S. (ksi)</th>
<th>0.2% Y.S. (ksi)</th>
<th>Elongation (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>min.</td>
<td>0.85</td>
<td>6.86</td>
<td>0.25</td>
<td>0.27</td>
<td>132.0</td>
<td>118.0</td>
<td>14.0</td>
</tr>
<tr>
<td>max.</td>
<td>0.93</td>
<td>10.08</td>
<td>0.74</td>
<td>0.67</td>
<td>143.0</td>
<td>130.0</td>
<td>18.0</td>
</tr>
<tr>
<td>average</td>
<td>0.88</td>
<td>8.46</td>
<td>0.47</td>
<td>0.47</td>
<td>137.2</td>
<td>124.9</td>
<td>15.7</td>
</tr>
<tr>
<td>standard deviation</td>
<td>0.02</td>
<td>0.84</td>
<td>0.14</td>
<td>0.12</td>
<td>3.3</td>
<td>3.5</td>
<td>1.4</td>
</tr>
</tbody>
</table>

Table 4.4: Statistics of the various input and output parameters in the tensile database for α+β forged samples (Bimodal Microstructure)
<table>
<thead>
<tr>
<th></th>
<th>Volume Fraction Total α</th>
<th>Globular Grain Size (µm)</th>
<th>α Grain Size</th>
<th>Volume Fraction Globular α</th>
<th>α Thickness in Transformed β (µm)</th>
<th>KQ (ksi (in)^1/2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>min.</td>
<td>0.34</td>
<td>9.19</td>
<td>0.13</td>
<td>0.15</td>
<td>61.3</td>
<td></td>
</tr>
<tr>
<td>max.</td>
<td>0.85</td>
<td>11.62</td>
<td>0.70</td>
<td>0.27</td>
<td>90.4</td>
<td></td>
</tr>
<tr>
<td>average</td>
<td>0.63</td>
<td>10.31</td>
<td>0.39</td>
<td>0.22</td>
<td>74.7</td>
<td></td>
</tr>
<tr>
<td>standard</td>
<td>deviation</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>standard</td>
<td>deviation</td>
<td>0.14</td>
<td>0.54</td>
<td>0.15</td>
<td>0.03</td>
<td>7.3</td>
</tr>
</tbody>
</table>

Table 4.5: Statistics of the various input and output parameters in the fracture toughness database for α+β forged samples (Bimodal Microstructure)
Figure 4.1: Schematics of thermomechanical treatment schedules baseline samples have undergone.
Figure 4.2: a) β-annealed microstructure b) β-Processed Microstructure
Figure 4.3: Stereological method to measure thickness of $\alpha$ laths.

Figure 4.4: Optical micrograph used in measuring the colony size factor. The black lines are randomly placed and the intercepts of the lines with the colony boundaries are marked with white circles.
Figure 4.5 Optical micrograph used in measuring the Prior β Grain Factor.

Figure 4.6: Stereology procedure for measuring volume fraction of α phase. A grid of points is laid down on the image and the white circles mark where the grid intercepts the β phase.
Figure 4.7: Stereology procedure for measuring volume fraction of basketweave region
Figure 4.8: Microstructure of a β annealed sample a) with small prior β grains; b) with large prior β grains
Figure 4.9: Microstructure of a β annealed sample a) with small size colony; b) with large size colony.
4.10: Microstructure of a β annealed sample a) with fully colony microstructure b) with mostly basketweave microstructure
Figure 4.11: Microstructure of a β annealed sample a) with thin α laths b) with thick α laths
Figure 4.12: Microstructure of a β annealed sample a) with small width of grain boundary α b) with large width of grain boundary α
Figure 4.13: Microstructure of α+β forged Ti-6Al-4V a) with small volume fraction of globular α b) with large volume fraction of globular α
Figure 4.14: Microstructure of $\alpha+\beta$ forged Ti-6Al-4V a) with small size of globular $\alpha$; b) with large size of globular $\alpha$
Figure 4.15: Microstructure of $\alpha+\beta$ forged Ti-6Al-4V a) with thin $\alpha$ laths in transformed $\beta$ region; b) with thick $\alpha$ laths in transformed $\beta$ region
4.16: Experimental Yield Strength values plotted against volume fraction of colony (all other microstructural features are varying too)

4.17: Experimental Yield Strength values plotted against Colony Size Factor (all other microstructural features are varying too)
4.18: Experimental Yield Strength values plotted against Prior $\beta$ grain Factor (all other microstructural features are varying too)

4.19: Experimental Yield Strength values plotted against $\alpha$ lath thickness (all other microstructural features are varying too)
4.20: Experimental Ultimate Tensile Strength (UTS) values plotted against Volume Fraction of Colony (all other microstructural features are varying too)

4.21: Experimental Ultimate Tensile Strength (UTS) values plotted against Colony Size Factor (all other microstructural features are varying too)
4.22: Experimental Ultimate Tensile Strength (UTS) values plotted against Prior β grain factor (all other microstructural features are varying too)

4.23: Experimental Ultimate Tensile Strength (UTS) values plotted against α lath thickness (all other microstructural features are varying too)
4.24: Experimental Elongation values plotted against Volume Fraction of Colony (all other microstructural features are varying too)

4.25: Experimental Elongation values plotted against Colony Size Factor (all other microstructural features are varying too)
4.26: Experimental Elongation values plotted against Prior $\beta$ grain factor (all other microstructural features are varying too)

4.27: Experimental Elongation values plotted against $\alpha$ lath thickness (all other microstructural features are varying too)
5.1 Regular Regression vs. Neural Network:

5.1.1 Linear Regression: Linear regression tools are familiar to the scientists and engineers. In linear regression, an estimate of the output (y) is obtained by the linear combination of a constant (θ) and products of each of the inputs (x_j) by a weight (w_j).

\[ y = \sum_j w_j x_j + \theta \]

w_j and θ are the best-fit parameter values (ie., for which the function best fits the data). Linear regression is a popular technique and there are many programs available which can perform linear regression (eg., MINITAB).

There are, however, disadvantages to using ordinary linear regression, some of which are as follows:

a) Linear regression is appropriate only if the data can be modeled by a straight-line function, which is often not the case.

b) Linear regression cannot easily handle categorical variables.

c) It is not easy to look for interactions between variables using linear regression.

d) The regression curve has the same form across the entire span of the input space.
5.1.2 Non-Linear Regression: Nonlinear regression extends linear regression to fit general (nonlinear) functions of the form:

\[ y = f(x_j, w_j) + \theta \]

Exponential or trigonometric functions used to model non-linear equations. There are many programs able to perform non-linear regression (e.g., NLREG). Although non-linear regression can capture non-linearity of output dependence on inputs there are several disadvantages of non-linear regression. They are as follows:

a) As with linear regression, nonlinear regression is not well suited for categorical variables or variables with interactions.

b) The form of the function has to be specified beforehand.

c) For complex inter-dependent data, it is very difficult to develop an appropriate non-linear model.

d) The regression curve has the same shape across the entire span of the input space.

5.1.3 Neural Networks:

Neural network modeling is a sophisticated method of non-linear regression that avoids the disadvantages mentioned with the other regression tools. It provides models of data relationships through interconnected and simulated “neurons” (nodes) that take inputs, apply weighting coefficients and feed their output to other nodes which then continue the process through the network to the eventual output. Neural Networks can be viewed as more flexible versions of traditional regression techniques. Because they are more flexible, they are able to fit the data better and model regularities in the data that
other regression models cannot capture. Neural networks are “trained” to deliver the desired result by an iterative process whereby the weights associated with each input at each node are adjusted to optimize the desired output.

Neural networks can model data that have complex non-linear relationships between the variables and can handle these interactions between the variables. Usually, hyperbolic tangent functions are chosen as the transfer function because of their flexibility. The strength of the hyperbolic tangent function is determined by the weight \( w_j \) and altering the weights can vary its exact shape. Also, it is to be noted that, as the hyperbolic function varies with the position in the input space, Neural Networks can capture the different complexities of the data at different positions across the span of input space. The degree of non-linearity present in a Neural Network is dependent on the number of hyperbolic tangent functions being used; varying this number permits the Neural Network method to capture almost arbitrarily non-linear relationships. The availability of sufficiently complex and flexible functions means that the Neural Network analysis is not as restricted as other regression tools, in which the form of the equation has to be specified before the analysis.

The neural network model can be used to examine the effect of an individual input on the output variable, whereas this may be incredibly difficult or in some cases impossible to do experimentally. The trend of the predicted output variation with an individual input variable (while keeping the values of the other variables constant) might guide us to a more physically based understanding. If any unexpected trend emerges from the models, it could point towards a previously unrecognized phenomenon. Examples of
how this has worked in this research will be discussed in later sections in which the results are discussed. In addition, a trained neural network can reveal the extent to which each input effects variations in the output variable.

To successfully use a neural network tool on a dataset, it is not necessary to have a prior knowledge of the physical phenomena associated with the data. Although the user does need to have some heuristic knowledge of how to select and prepare data, how to select an appropriate neural network, and how to interpret the results, the level of user knowledge needed to successfully apply neural networks is much lower than would be the case when using, for example some more traditional nonlinear statistical methods.

5.2 Neural Network Basics and Bayesian Interpretations:

For the present research, a probabilistic Bayesian neural network architecture developed by Mackay[91] has been used to develop a microstructure-based mechanical properties models for Ti-6Al-4V. For developing a microstructure-based mechanical property model using neural networks, a database is first populated with quantified values of microstructural features and the tensile properties. The microstructural features are the input variables and the mechanical properties are the output (or target) variables.

When a dataset is obtained, it is first divided into two sets, the training and test set. In the present case, approximately 33% (or sometimes a smaller fraction) of the data from the original database were chosen randomly to form the test set. Although the selection of the test set is random, care is taken to ensure that the training set includes some data having the extreme values for all input and target variables. The network is
trained using the training dataset and is tested for its capability of generalization on the test data. Both the input and the target variables are first normalized within the range +/- 0.5 with respect to their extreme values as follows:

\[ x_N = \frac{x - x_{\text{min}}}{x_{\text{max}} - x_{\text{min}}} - 0.5 \]  

(1)

where \( x_N \) is the normalized value of \( x \), \( x_{\text{max}} \) is the maximum value and \( x_{\text{min}} \) is the minimum value of each variable in the dataset. Normalization of the variables is not essential, but it is done because it makes the search for optimal parameters easier during training and it facilitates the subsequent comparison of the significance of each of the variables [92].

In mathematical terms, the training dataset is a set of input-target pairs \( D = \{x^m, t^m\} \) where \( m \) is a label denoting the different input, target pairs [93]. A neural network architecture, \( A \) is described by the number of layers, number of nodes in each layer, type of activation function performed by each node and the weights \((w)\) and biases \((\theta)\) associated with each connection. The set of all the weights and biases of the network makes up the weight vector \((w)\). Once the architecture is defined and a set of values \( w \) is assigned to the connections between the nodes, then the network produces the output value \( y(x^m; w) \) from the input values \( x^m \). The differences between the output predictions of the network and the target values is described by an error function,

\[ E_D(w) = \frac{1}{2} \sum_m (y(x^m; w) - t^m)^2 . \]  

(2)
$E_D$ is minimum when the network fits the training data well, i.e., when $y(x^m; w)$ approximates $t^m$.

A typical neural network architecture is shown in the figure 5.1 [94]. This is a 3-layer feed forward type network. It has one hidden layer between the input and output layers. In the input layer, the nodes denote input variables ($x_j$) and the output node denotes the output variable ($y$). The transfer function relating the input to the $i^{th}$ hidden node is given by

$$h_i = \tanh\left( \sum_j w_{ij} x_j + \theta_i \right).$$

i.e., linear functions of the inputs $x_j$ are operated on by a hyperbolic tangent transfer function. The transfer function relating hidden nodes to the output is linear given by

$$y = \sum_i w_i^{(2)} h_i + \theta^{(2)}.$$

With some initial values of the weight vector ($w$), the network predicts the value of the output variable ($y$). During the training, the values of weights ($w$) and biases ($\theta$) are constantly readjusted in different iterations to minimize the objective function given by[95]

$$M(w) = \beta E_D + \sum_c \alpha c E_{w(c)}.$$

The objective function ($M(w)$) is a function of the weight vector ($w$), and it contains an error function term $E_D$ given by equation (2) as well as some regularizer terms $E_{w(c)}$ which favor small values of $w$ and decrease the tendency of the model to overfit noise in the training data. The regularization method used here is known as the
Automatic Relevance Determination method [96]. Each weight is assigned to a class (c) depending on the connection it is associated with. Weights connected from an input node to all the hidden nodes are in a single class. Hidden node biases are in their own class, and all the weights from the hidden nodes to the output node are in another class. \(E_{w(c)}\) is defined to be the sum of the squares of the weights in class c, and can be calculated as follows:

\[
E_{w(c)}(w) = \frac{1}{2} \sum_{i \in c} w_i^2.
\]  

(6)

The hyperparameters, \(\alpha_c\) and \(\beta\) are known as control parameters. The Bayesian neural network is given a probabilistic interpretation, which involves assigning a meaning to the functions and the parameters, according to which the hyperparameters define the assumed Gaussian noise level \(\sigma_v^2 = \frac{1}{\beta}\) (\(\sigma_v\) is the noise level inferred by the model) and the assumed weight variances \(\sigma_{w(c)}^2 = \frac{1}{\alpha_c}\). Denker and LeCun have given a simplistic view of this probabilistic interpretation of the neural network. In their model explanation, the input-output relation of the network is given a probabilistic distribution \(P(O, I)\) (rather than the usual function \(O = f(I)\)) where O and I are the output vector and input vector, respectively.

Under this probabilistic framework, the weight vector \(w\) is a set of probability distributions and the minimization of \(M(w) = \beta E_D + \sum_c \alpha_c E_{w(c)}\) is identical to finding the
local values for the most probable parameters $\mathbf{w}_{MP}$. The objective function $M(\mathbf{w})$ is minimized by an efficient optimization technique, the “variable metric method”\cite{96}. The optimization of $M$ treats all data points equally irrespective of the order in which they are located in the database since $E_D$ is defined as the error on the entire training dataset. The training dataset is used to optimize the weight parameters ($\mathbf{w}$) of the network and the test dataset is used to optimize the control parameters such as $\alpha$ and the network architecture $A$.

As described earlier, because there is a probability distribution on $\mathbf{w}$, there is an associated probability distribution on the output, even for fixed inputs. Denker et. al.\cite{97} described how the variance of the output distribution allows one to place error bars on the output confidence. The variance of the output distribution has two components; one is the variance of the assumed Gaussian noise level of the training data and second is the variance on the output. Once the most probable values for the range of weights ($\mathbf{w}_{MP}$) are determined, the sensitivity of the output (say it is denoted by $\mathbf{g}$, where $g_i = \frac{\partial y}{\partial w_i}$) to any uncertainty in the weight space (holding the input set fixed) and the curvature (double gradient or Hessian, denoted by $A$) of the objective function $M(\mathbf{w})$ at the most probable value of weight vector ($\mathbf{w}_{MP}$) are calculated. These are used to find the variance-covariance matrix ($g^TA^{-1}g$) for the output \cite{98}; the square root of the corresponding diagonal element of this matrix is taken to estimate the error bars on a single prediction. The result is a network that produces not only a “best guess” output value corresponding
to the most probable values of weights but also an “error bar” which indicates the confidence interval around that output.

5.3 Brief Description of Bayesian Probability Theory:

In this section, the basics of Bayesian probability theory as elaborated in MacKay’s [99] and other researchers’ work will be discussed in brief.

What is effectively done when modeling data is translating statistical sample data into generalizations, usually with a calculated degree of certainty; this is called inference. There are two distinct levels of inference in the case of regression with different models; namely; these levels are “model fitting” and “model comparison”. In Model Fitting, a particular model $H_i$ is assumed to be true, and the values for the model’s parameters, $w$ are inferred from the data $(x, t)$. In more precise terms, by model fitting the most probable values of the parameters as well as their one-standard-deviation errors are inferred for a particular model. The second level of inference is the task of model comparison, in which some sort of ranking or preference is given to the alternative models ($H_i$ ’s are different models).

A model $H_i$ is defined by a collection of probability distributions: a ‘prior’ distribution $P(w | H_i)$ which states what the values model’s parameters might plausibly take, and a set of probability distribution for each value of $w$, which define the predictions $P(t | x, w, H_i)$ that the model makes about the data $(x, t)$. So, when a particular model $(H_i)$ is specified, the probability distributions, $P(w | H_i)$ and
$P(t \mid x, w, H_i)$ are known. These probabilities are known respectively as the prior probability distribution of parameters and the likelihood (or prediction on the data).

5.3.1 Model Fitting: Using Bayes’ rule, the posterior probability of the parameters $w$ is first inferred as follows:

$$P(w \mid x, t, H_i) = \frac{P(t \mid x, w, H_i)P(w \mid H_i)}{P(t \mid x, H_i)} \quad (7)$$

The probability distribution $P(t \mid x, H_i)$, known as the evidence, acts just as a normalizing constant in this equation and is ignored because it is irrelevant for the inference of values for $w$. Using gradient based methods, the maximum of this posterior probability which defines the most probable value for the parameters is found and labeled $w_{MP}$. The posterior distribution is summarized by the value of $w_{MP}$ and its error bars.

5.3.2 Model Comparison: At the second level of inference, models are assigned ranks in the presence of data ($x$, $t$). The posterior probability of each model, $H_i$ is:

$$P(H_i \mid x, t) \propto P(t \mid x, H_i)P(H_i) \quad (8)$$

First term on the right hand side, $P(t \mid x, H_i)$ is the evidence for $H_i$. The second term, $P(H_i)$ is the subjective prior which expresses how plausible the alternative models were thought to be in the absence of the data. If it is chosen to assign equal priors ($P(H_i)$) to alternative models, then the models $H_i$ are ranked by evaluating the evidence. So, in order to assign a preference to alternative models, the Bayesian framework evaluates the evidence $P(D \mid H_i)$.
The next step is to evaluate this evidence, \( P(t \mid x, H_i) \). As mentioned earlier, the evidence is the normalizing constant for the equation of the posterior probability of the parameters. So, the evidence is found by integrating the numerator of the equation for posterior as follows:

\[
P(t \mid x, H_i) = \int P(t \mid x, w, H_i)P(w \mid H_i)dw \tag{9a}
\]

Now as the posterior of parameters, \( P(w \mid x, t, H_i) \propto P(t \mid x, w, H_i)P(w \mid H_i) \), the above equation can also be written as \( P(t \mid x, H_i) \propto \int P(w \mid x, t, H_i)dw \), and as the posterior usually has a strong peak at the most probable parameters, \( w_{MP} \), with a characteristic width, \( \sigma_{wD} \) (see figure 5.2 [99]), the above integration can be approximated as

\[
P(t \mid x, H_i) \approx P(w_{MP} \mid x, t, H_i)\sigma_{wD} \text{ (i.e., height multiplied by the width of the integral).}
\]

So, the evidence becomes

\[
P(t \mid x, H_i) \approx P(t \mid x, w_{MP}, H_i) \times P(w_{MP} \mid H_i)\sigma_{wD} \tag{9b}
\]

The quantity \( \sigma_{wD} \) is the posterior uncertainty in \( w \). If for simplicity the prior \( P(w \mid H_i) \) is supposed to be uniform on some large interval \( \sigma_w \) (see figure 5.2), then

\[
P(w_{MP} \mid H_i) = \frac{1}{\sigma_w}, \text{ so that the evidence becomes}
\]

\[
P(t \mid x, H_i) \approx P(t \mid x, w_{MP}, H_i) \times \frac{\sigma_{wD}}{\sigma_w} \tag{9c}
\]

The first term in the right hand side of this equation is the “Best fit likelihood” and the second term, which is the ratio of the posterior width (after the data arrived) to the prior width (before the data arrived) is known as the “Occam factor”. The Occam factor
penalizes the more complex models in the following way. A complex model having many parameters, each of which is free to vary over a large range $\sigma_w$, will have a small Occam factor resulting in a smaller value for the evidence of that model compared with a simpler model. This is illustrated in figure 5.3 [99]. A simple model $H_1$ makes only a limited range of predictions. The more powerful model $H_2$, having more free parameters, predicts a greater variety of datasets. In the dataset region $C_1$, the less powerful model $H_1$ will be the more probable model.

In summary, Bayesian probability theory automatically embodies Occam’s razor, a philosophy stating a preference for the simpler model. Alternative models are ranked by their evidence values; which model recurs the greatest evidence is then determined by a trade-off between minimizing the natural complexity measure (minimizing $\sigma_w$) and minimizing the data misfit (or maximizing the likelihood, $P(t \mid x, w_{MP}, H_i)$).

5.4 Bayesian Probabilistic Interpretation of the Neural Network Objective Functions:

MacKay has explained how the objective functions are given a Bayesian Probabilistic interpretation [99]. This will be briefly discussed in this section.

The sum square error, $E_D$ in equation 2 is assumed to correspond to Gaussian noise on target variables, where the parameter $\beta$ defines a noise level $\sigma_v^2 = \frac{1}{\beta}$. The error function $E_D$ is then interpreted as minus the log likelihood for an overall data-noise level as
Similarly, the prior distribution is assumed to be Gaussian with a variance \( \sigma^2_w = \frac{1}{\alpha} \). \( E_w \) in equation 6 then interpreted in terms of log prior distribution as follows:

\[
E_w = -\frac{1}{\alpha} \ln(z_v(\alpha)P(w|\alpha,H_i)).
\]  

(11)

The objective function then corresponds to the inference of parameters \( w \) (posterior probability of parameters):

\[
P(w|x,t,\alpha,\beta,H_i) = \frac{P(t|x,w,\beta,H_i)P(w|\alpha,H_i)}{P(t|x,\alpha,\beta,H_i)} = \frac{1}{z_M} \exp(-M(w)),
\]

which implies the objective function in the equation 5 is interpreted as:

\[
M(w) = -\ln(z_M P(w|x,t,\alpha,\beta,H_i)).
\]  

(12)

As mentioned earlier, by training the neural network this objective function \( M(w) \) is locally minimized to obtain the most probable parameter vector, \( w_{\text{MP}} \).

5.5 Advantages of Bayesian Neural Networks:

A common problem with the use of powerful non-linear regression or other statistical neural network tools is the possibility of overfitting the data. Using Bayesian methods in Neural Network modeling solves this overfitting problem by controlling the model complexity. Bayesian model comparison embodies Occam’s razor, the principle that states a preference for simple models [96]; the Bayesian Occam’s razor automatically suppresses the tendency to fit the spurious structure of the data.
Bayesian model comparison can be used to optimize weight decay rates and to automatically infer which are the relevant input parameters for a problem. It is to be noted that, as the model comparison in Bayesian framework is done by calculating the evidences for alternative models, which does not involve a “testing” or “validation set”, all available training data can be devoted to both model fitting and model comparison. For a large test data set, the correlation between the test error and the evidence for alternative models is good, and often the test error is used for the selection of better models.

Probabilistic modeling in the Bayesian framework handles the uncertainty in a natural manner. The probabilistic nature of Bayesian network incorporates uncertainty about parameters into predictions of other variables uniquely.

As described in the previous section, Neural Networks in a Bayesian framework allow for the calculation of error bars to represent the uncertainty in the fitting parameters. Instead of calculating a unique set of weights, a probability distribution of sets of weights is used to define the fitting uncertainty. As a result, the error bars become large when data are sparse or locally noisy.

5.6 Fuzzy Logic Neural Networks:

Fuzzy logic systems are developed to solve complex problems which are ill-defined and difficult to mathematically analyze [100]. In fuzzy systems, functions are estimated by the linguistic association between inputs and outputs; i.e., their inter-relationship is defined by if-then statements. Fuzzy logic uses a continuous range of truth
values in the interval [0,1] rather than a strict binary (True or False) decisions and assignments [101]. Fuzzy rules-based systems apply these methods to solve many types of "real-world" problems, especially where a system is difficult to model, is controlled by a human operator or expert, or where ambiguity is common. A typical fuzzy system consists of a rule base, membership functions, and an inference procedure (see Figure 5.4) [101]. In fuzzy-logic based solutions, inputs are first fuzzified (crisp to fuzzy) using membership functions, and are then operated on by rules-based approaches to infer the output, which in the last step is then defuzzified.

The key benefits of fuzzy design are as follows [101]:

a) They are easy to implement.

b) They involve a simplified & reduced development cycle

c) They can provide more "user-friendly" and efficient performance.

In our present research, a commercial software package named “CubiCalc RTC 2.0” marketed by Heperlogic Corporation has been used. CubiCalc uses fuzzy logic to implement a neural network. In CubiCalc, rules are developed using a module named “Rule Maker” to solve the regression problem by fuzzy logic. This is a user-friendly tool; however, the software is limited in the number of inputs and outputs it can use in a model. As a result, it can not always capture the real complexity present in the problem.

5.7  Limitations of Neural Networks:

Neural Networks have few limitations. Neural Networks are completely database dependent. The quality and quantity of the data in the training dataset largely affect the
predictive performance of a Neural Network on unseen data; a few spurious data in the training dataset can negatively affect its performance. An overly flexible network may try to fit to a non-existing trend because of some stray data. The performance of a network can be sensitive to the quality and type of preprocessing of the training data.

The neural network method cannot cope with missing values. As a result, an over ambitious choice of input variables will in general limit the number of complete set of data available for training. On the other hand, neglect of an important input variable leads to an increase in the noise associated with predictions [102]. So, the number of inputs chosen is a compromise between the definition of the problem and the availability of data.

Neural Networks are not always the best tools applicable for a prediction problem. Before one starts a simulation using a neural network, one should try to find out whether alternative methods exist and if a neural network can treat the given task. It is, for instance, not a good idea to try to predict the results of the next lottery drawing based on the last five drawings using neural networks, because one cannot expect any correlations between the different drawings. In many situations, one expects correlations between data but one does not know any rules or laws that could be used for a prediction. Such a situation is ideal for the application of a neural network.
Figure 5.1: Schematic of a 3-layer neural network

Figure 5.2: The Prior distribution (solid line) for the parameter has width $\sigma_w$. The posterior distribution (dashed line) has a single peak at $w_{MP}$ with characteristic width $\sigma_{w|D}$. The Occam factor is $\frac{\sigma_{w|D}}{\sigma_w}$. 

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Figure 5.3: Bayesian inference embodies Occam’s razor. Simple model $H_1$ makes only a limited range of predictions. More powerful model $H_2$ (more free parameters) predicts a greater variety of datasets.

Figure 5.4: Schematic of a Fuzzy Solution path
6.1 **β**-Heat-treated Ti-6Al-4V with colony/basketweave microstructures:

### 6.1.1 Identification and sensitivity analysis of important microstructural features:

Based on initial experiments with Fuzzy Logic neural networks, four microstructural features were determined to be the most important in terms of influencing the tensile properties in β-heat-treated colony microstructure in α/β Ti alloys. They are: thickness of the α laths, volume fraction of total α, colony size, and prior β grain size.

As mentioned earlier, measurement of both the colony size and prior β grain size requires knowledge of their shape. However, these features have complicated shapes that cannot be easily characterized or generalized. Using stereological methods, these features are measured quantitatively without assuming any shape and are represented by size factors. The colony size measured in this way is represented by the colony size factor, which conceptually is the average length of a randomly oriented line (in three dimensions) that intersects the colony [87]. The colony size factor has a dimension of length that represents the colony size; it is termed as “size factor” because it does not give any information regarding the shape of the colonies. In contrast, the prior β grain size is
indirectly measured by measuring the surface area per unit volume of the grains, and is termed the prior $\beta$ grain factor. It is to be noted that the prior $\beta$ grain factor has a dimension of the reciprocal of length; the larger the value of the prior $\beta$ grain factor, the smaller the prior $\beta$ grain size is.

The database contains values for the thickness of $\alpha$ lath, volume fraction of total $\alpha$, colony size factor and prior $\beta$ grain factor, which will be used as input parameters, and the tensile properties (yield strength, ultimate tensile strength and elongation) as output parameters. Table 4.1 lists the range, average, and standard deviation for the values in the two databases. Because of the relatively small population in the database (86 data points), 70 samples have been chosen for training the Bayesian Neural Network and 16 samples for testing and validation of the network performance. Test data-points are randomly chosen from the database. After training the network, the significance of each of the input variables as perceived by the model can be obtained; it is given by the Gaussian width ($\sigma_w$) corresponding to each individual input variable and is shown in figure 6.1. The parameter $\sigma_w$ is similar to a partial correlation coefficient in that it represents the amount of variation in the output that can be attributed to any particular input variable. From figure 6.1 it is seen that, for this database, $\alpha$ lath thickness and prior $\beta$ grain size are two microstructural input variables that appear to significantly affect the yield strength of Ti-6Al-4V.
6.1.2 Prediction of properties:

After training, the network has been used to predict the tensile properties. Figure 6.2, 6.3 and 6.4 show the predictions of yield strength, ultimate tensile strength and % elongation for 16 test data points. The dashed line is the zero error line and the solid lines are +/- 5% error lines. It is seen that the trained neural network is able to predict the yield and ultimate tensile strength values of Ti-6Al-4V from the microstructural features within +/- 3 % and +/- 4% error respectively. Its ability to predict elongation is not as accurate as for the tensile strengths. It is of interest to identify the factors that limit the accuracy of these predictions. Because the approach used here essentially involves non-linear regression, it is immediately obvious that the accuracy may be improved by the use of a larger database population. In addition, it is important to consider whether important microstructural features have not been included in the analysis. For example, the effects of local texture differences have not been quantified and included in the model. Also, the oxygen concentration, which is thought to harden $\alpha$-Ti, has not been measured. If effects such as these are taken into account, the observed accuracy may increase, and this is under the scope of further research.

The model’s accuracy for predicting elongation is much lower than for the tensile strength; this might because the elongation at failure of the sample has been used in the model. However, after necking begins, the material deformation is unstable and cannot be related to microstructure as well as the properties in the stable deformation zone. It is suggested that the % elongation can be more accurately predicted on the microstructural features if the elongation until the necking point is measured and modeled [103].
6.1.3 Virtual Experiments:

In addition to their promising predictive capability, neural networks can also be used to extract the functional dependencies of the tensile properties on individual microstructural features. These dependencies can guide the development of a physically based model for the property-microstructure relationship. While it is experimentally impossible to vary one particular microstructural feature independent of all others, virtual experiments can be performed using trained neural networks whereby each individual microstructural parameter can be varied without changing the values of the others. For example, while the variation in yield strength as a function of $\alpha$ lath thickness is plotted in Figure 6.5 for various samples, it should be noted that the values of other microstructural features such as colony size factor, prior $\beta$ grain factor and volume fraction of total $\alpha$ are also simultaneously changing due to their interdependent response to the given heat treatment. As a result, it is not possible to obtain an independent trend of YS variation with $\alpha$ lath thickness. A solution involves the use of the trained neural network to perform virtual experiments. In this way, properties can be predicted as a function of the value of the microstructural feature of interest while keeping the other microstructural input parameters at constant values within their experimental range. Such a trend plot has been demonstrated in Figure 6.6 for the variation of YS with thickness of $\alpha$ lath, where the values of the other microstructural parameters (volume fraction of total $\alpha$, colony size factor and prior $\beta$ grain factor) are kept constant at their mean values in the training database. From this trend plot, it is expected that the YS would decrease
monotonically with increasing $\alpha$ lath thickness. Similarly, the trend plot in Figure 6.7 shows a monotonic decrease in YS with increase in colony size, but the effect is not as large as that of the $\alpha$ lath thickness. A moderately positive effect of volume fraction of the $\alpha$ phase on YS is illustrated in Figure 6.8.

These trend plots for the variation of strength with individual microstructural parameters are consistent with the expected behavior. For example, with decreasing thickness of the $\alpha$ laths, the effective slip length decreases, and so based on dislocation pileup lengths, the yield strength should vary inversely with the $\alpha$ lath thickness. The trend plot produced by the neural network shown in Figure 6.6 correctly predicts this behavior. Similarly, the neural network also predicts an inverse trend for yield strength with colony size. In this case, the strength effect of the colonies can also be rationalized based on the slip length argument [104,105,85]. The Burgers orientation relationship that exists between the $\alpha$ and $\beta$ phases within a single colony allows for an easy slip transfer across the $\alpha/\beta$ boundary. Because the $\alpha$ laths within a single colony are all similarly oriented, slip can easily traverse the entire colony. This should make the colony size a significant microstructural dimension affecting the yield strength in this alloy. Once again, the trend plot predicted by the neural network shown in Figure 6.7 correctly predicts this behavior, although the predicted trend is less significant when compared with the effect of lath thickness on yield strength. This may be due to the increased number of $\alpha/\beta$ boundaries afforded by decreasing $\alpha$ lath thickness for the same colony size. Thus, although it has been previously assumed [85] that slip transfer across $\alpha/\beta$
boundaries is relatively easy, these boundaries may offer more resistance to slip transfer than previously considered. This is promising for further research.

The amount of total $\alpha$ in the microstructure appears to have a moderately positive effect on YS within the limits of the test matrix. This might be expected, since the $\alpha$ phase is stronger than the $\beta$ phase.

Finally, the effect of prior $\beta$ grain size on YS is of interest. The prior $\beta$ grain size, in general, is believed to have a minimal influence on YS of Ti-6Al-4V alloys [21]. However, the trend plot predicted by the neural network, using the industry provided samples in this study, shows a positive impact of the prior $\beta$ grain size on the YS (Figure 6.9). This direct relationship between the prior $\beta$ grain size and the YS is somewhat unexpected and counterintuitive, since refining the grain size is expected to be associated with an increase in strength. Because of this unexpected behavior, the microstructures of the samples yielding small and large prior $\beta$ grain sizes were further studied. These detailed investigations of the microstructures led to two broad categories of prior $\beta$ grain structure based on their original grain size as shown in Figure 6.10. Smaller prior $\beta$ grains ($< 200 \, \mu m$) contained uniform colony microstructures. In contrast, the microstructure of large prior $\beta$ grain consisted of a mixture of colony and basketweave microstructures. A colony microstructure was seen to form near the grain boundaries, whereas basketweave microstructures were prevalent in the interior of larger grains. Based on above findings, the data set was grouped into two broad categories based on the prior $\beta$ grain factor and trend plots predicted by the neural network were recalculated. In Figure 6.11, the YS has
been plotted against the prior $\beta$ grain factor for these two separate databases. The trend plot from the fine grain material shows a smaller dependence of the prior $\beta$ grain size on the YS than the trend plot corresponding to the larger grain samples. It appears that a significant variation of YS with the prior $\beta$ grain size occurs in samples with large grains, where the basketweave microstructure is expected to make up a significant fraction of the material. Hence, it is important to include a new microstructural feature, namely the fraction of basketweave microstructure, in the neural network model.

After recognizing the basketweave microstructure as another important feature with respect to its effect on the strength of Ti-6Al-4V alloy, additional characterization of the samples was undertaken to quantify the individual volume fractions of basketweave and colony microstructures. The volume fraction of basketweave microstructure was then used as an additional input parameter to the neural-network modeling. Figure 6.12 shows the YS variation with the prior $\beta$ grain factor obtained by re-training the database using the volume fraction of basketweave as an additional input parameter. This plot is markedly different from our earlier predictions (Figure 6.9 and 6.11), and shows a negative effect on YS as expected. This analysis highlights the usefulness of the approach to use neural networks to identify significant microstructural features and improve the understanding of microstructure-property relationships upon which mechanistic models can then be based. This variation in YS with prior $\beta$ grain size as depicted in figure 6.11 was known previously but not understood. Neural network modeling has permitted an understanding to be developed.
Variations in elongation with individual microstructural variables are shown in figures 6.13 through 6.16. The elongation is found to increase with an increase in the thickness of α laths; but it decreases with increasing colony size and prior β grain size. The volume fraction of total α doesn’t appear to have any effect on the % elongation. The colony size effectively determines the slip length; with refining colony size, the slip length decreases and less stress concentration builds up along the colony boundaries, decreasing the chance of crack initiation, and increasing the ductility of the material.

6.2 β annealed Ti-6Al-4V with colony/ basketweave microstructures:

In the previous section, neural network models have been discussed for β heat-treated Ti-6Al-4V samples, which include both β processed (worked above the β transus, but no subsequent heating above the β transus) and β annealed (worked above or below the β transus, with subsequent heating above the β transus) samples. Schematics of these two types of thermomechanical treatments are shown in figure 4.1. The microstructures generated by these two types of thermomechanical schedules have been discussed in chapter 4. The β processed samples have a more deformed microstructure; in industry, the β anneal treatment is usually applied for Ti-6Al-4V as opposed to the β process treatment. It was therefore suggested in an MAI meeting that the tensile properties models be developed for only the β-annealed samples. Accordingly, β annealed samples were separated out from the database to make a new database of β annealed samples whose statistics has been given in table 4.2. It should be noted that the volume fraction of
total α has been taken out from the input variables list and replaced by volume fraction of basketweave/ colony.

6.2.1 Optimized architecture of the trained networks and Property Predictions:

Out of the data from the 52 β-annealed samples, 17 data-points were randomly chosen as test data points and the remaining 35 data points were used for training (optimizing the weight vector for each architecture).

Test data are used to optimize the model architectures. Based on training of the yield strength model, the optimized committee model was in fact a combination of two different network architectures. The values of seed, number of hidden nodes and initial Gaussian width for these two models in the committee model can be written as $10^4$, 4, 1.0 for the first model; and 100, 4, 0.01 for the second model. The trained network’s performance is shown in figure 6.17, where the predicted yield strength has been plotted against the experimental yield strength for the test data points. Most of the data are pretty close to 0-error line. The predicted values are given along with their corresponding error-bars, which are the confidence interval (+/- one standard deviation) on the best guess output values.

For the ultimate tensile strength model, the optimized model architecture was found to have the following values of seed, number of hidden nodes and initial Gaussian width: $10^5$, 4 and 3.0 respectively. Predictions of the ultimate tensile strength for these β-annealed samples are shown in figure 6.18. Again, the predictions are plotted along
with their corresponding error-bars. These predicted values are for randomly chosen test data points and are seen to fall well within the +/- 5 % error lines.

The elongation prediction model has been optimized for a combination of two different network architectures. The values of seed, number of hidden nodes and initial Gaussian width for these two models in the committee model can be written as $10^6$, 4, 1.0 for the first model; and $10^4$, 3, 5.0 for the second model. The performance of this committee model is shown in figure 6.19. The prediction of elongation is not as good as for the strength properties. As discussed in an earlier section, a probable reason for this is that this research the elongation at failure (which is a parameter characteristic of unstable plastic deformation zone of stress-strain diagram) has been modeled based on the microstructure of the undeformed material (where the material has not been deformed plastically in an unstable way, i.e., the microstructure before necking).

6.2.2 Design Tool & Trend Plots:

In order to make these neural network models more user-friendly, two approaches have been taken. One is to make spreadsheets with the proper equations and weight parameters, where the users need only to enter the values of the input variables and obtain the tensile property value. The second is to develop a JAVA-based design tool, where the user can change or set the values of input variables by moving the slide bars or entering values in the boxes, and can see how the value of the tensile property changes online. In the design tool one can see the trend plots of tensile properties with individual microstructural features while other microstructural features are set constant at any value.
in their ranges by the user. Figures 6.20, 6.21 and 6.22 show the spreadsheet version of the end-user tool for yield strength, ultimate tensile strength and elongation prediction. In the spreadsheet, one can enter the values of microstructural features for a sample whose property values are needed and get the property value.

An advanced design tool based on JAVA coding (Coding done by Dr. Samrat Goswami, Post Doctoral Fellow, University of Texas, Austin) has been developed for mechanical property predictions and trend plots based on the microstructures of Ti-6Al-4V. Figure 6.23 and 6.24 show snapshots of such a design tool for yield strength and ultimate tensile strength of β annealed Ti-6Al-4V samples. From the trend plots, it is seen that both the yield strength and tensile strength increase as the volume fraction of basketweave in the microstructure increases. The importance of basketweave microstructure on the strengths of α/β Ti alloys has been identified for the first time as described earlier in this chapter. Both the yield strength and tensile strength are seen to increase with decreasing size of the colonies, prior β grains and α lath thickness. These trends are similar to β heat-treated samples, and have been discussed in detail in a previous section. Figure 6.25 shows a snapshot of the design tool for elongation of β annealed Ti-6Al-4V. Elongation is found to increase with an increase in volume fraction of colony in the microstructure. This trend is similar to that of the toughness variation with volume fraction of colony (discussed in next chapter). So, while the volume fraction of basketweave region is considered to be beneficial with respect to the strength of the material, it adversely affects the ductility and toughness of β annealed Ti-6Al-4V. Ductility (measured by % elongation) increases with decreasing size of the colonies in
the microstructure; the colony size determines the effective slip length of this material microstructure, so as the colony size decreases the slip length decreases. This in turn causes the number of dislocations in the pile ups to decrease causing a smaller stress concentration in the material, which manifests itself in the increased elongation values with decreasing colony sizes. Thicker α laths appear to result in more ductility. The physical reasoning behind these trends could be a topic for further research.

6.3 Predictive models for Mechanical Properties based on Processing Parameters:

While developing microstructure-based property models, a brief effort was made to see how the processing parameters could be used in predicting the mechanical properties. The results will be presented in this section. Processing parameters for both β heat-treated and α+β processed samples were used as the input variables to the neural network, and mechanical properties were used as the output. 7 input variables were used. They are: the Forge Temperature, the Strain Level applied during forging, the Orientation (Axial or Radial in case of the tensile samples and L-R or R-L in case of the toughness samples), the Solution Temperature, the Cooling Rate (cooling down from the solutionizing temperature), Age Temperature and Age Time. Quantitative data were available for the temperature, time and strain variables but not for the orientation. However, because the neural network only takes quantitative data, the orientation data, such as Axial or Radial for the tensile samples, has been represented in the network as 1 or 0 respectively; similarly, for the toughness data, L-R and R-L orientations have been represented in the network as 1 and 0 respectively. There were 120 samples total
(including both the β heat-treated (86 samples) and the α+β processed (34 samples)) in the database. From this dataset, 22 data (which includes 16 β heat-treated and 6 α+β processed samples) were randomly chosen to make the test set. The ranges of the values of thermomechanical variables used for processing the samples have been discussed in the Database Development Chapter (Chapter 4). After training, the performance of the networks was shown by plotting the predicted mechanical properties (network outputs) against the experimentally obtained mechanical properties data (target values). Figure 6.26 shows the predicted yield strength for the test data points based on the processing parameters. The blue diamond points are data points for the β heat-treated samples and the red triangular points are for the α+β processed samples. Similarly, predicted values for other mechanical properties (ultimate tensile strength, elongation, reduction in area and toughness) are shown in figures 6.27 through figure 6.30. It is observed that, while the yield strength and ultimate tensile strength predictions are impressively accurate, predictions of the elongation, reduction of area and fracture toughness are not as good.

Although the present research effort is focused on the development of microstructure-based property models, a few processing variables can be used along with microstructural variables as inputs. For example, in the case of the α+β processed bimodal microstructure, to capture the effect of tertiary fine α laths, which develop during aging heat-treatment, age temperature and age time can be used as two additional input variables along with microstructural variables (volume fraction of total α, volume fraction of globular α, size of globular α, and α lath thickness in transformed β). At present, a measurement procedure for these fine scale tertiary α laths in the transformed β
region has not been standardized, one way to include this microstructural feature is to include age temperature and age time as two additional input variables. These fine scale α laths are precipitated during an ageing heat-treatment, and their dimensions are a function of the aging parameters. This is promising for further research.

6.4: Neural Network model for tensile properties of α+β processed bimodal microstructures:

When α/β titanium alloys, such as Ti-6Al-4V, are mechanically worked/deformed heavily in the α+β phase field, then a bimodal microstructure consisting of both the globular α phase and the colony/basketweave region known as the transformed β region is formed. This has been discussed in detail in the Background and Literature Review chapter (Chapter 2). Figure 6.31 shows microstructures of two extreme yield strength samples; one (figure 6.31a) with a low yield strength and the other (figure 6.31b) with a higher yield strength. The obvious microstructural differences are in the volume fraction of globular α and the thickness of α laths in transformed β. Therefore, these two microstructural features along with the size of globular α and volume fraction of total α have been identified to be the most important microstructural features guiding the tensile properties in α+β processed Ti-6Al-4V samples. These microstructural features were characterized and quantified values of them were obtained using stereological procedures. The range, average and standard deviations of the microstructural variables and tensile properties are shown in table 4.4. Microstructural variables were input to the neural network, and tensile properties were generated as the output of the network. There
were a total of 136 data points in the database, 36 of which have been randomly chosen to be in the test data set. The performance of the trained network is shown in figure 6.32, where the predicted yield strength has been plotted against experimentally obtained yield strength for the test data points. As before, predicted values are given along with error bars (+/- one standard deviation around the best guess output value). Predictions on the test data points are within +/- 5 % error.

Virtual experiments were performed whereby the effects of individual microstructural features on yield strength could be seen. Figure 6.33 and figure 6.34 are two snap shots of the design tool made for yield strength of bimodal microstructures. In the design tool, a person can obtain not only the value of yield strength for a particular combination of microstructural features values, but can also see the trend plots for variations of yield strength with individual microstructural features when other microstructural features are kept constant at some particular values in their range. Figure 6.33 shows a monotonic decrease of the yield strength with volume fraction of globular \( \alpha \) and with \( \alpha \) lath thickness in transformed \( \beta \), along with increase in yield strength with increasing volume fraction of total \( \alpha \) and size of globular \( \alpha \). Based on the plots given by this tool, one could determine that, to produce a high strength material, one needs a material whose microstructure has a low volume fraction of globular \( \alpha \) and thin \( \alpha \) laths in transformed \( \beta \) region. The increasing trend of yield strength with the volume fraction of total \( \alpha \) is due to the presence of more of the stronger \( \alpha \) phase. Figure 6.34 shows that the trend for yield strength variation with the size of globular \( \alpha \) changes from increasing to decreasing as the thickness of \( \alpha \) laths in transformed \( \beta \) is kept constant at larger values.
(thick \( \alpha \) laths) instead of small values (thin \( \alpha \) laths). This is an interesting observation and might be due to a change in strengthening mechanism accompanied by a change in the thickness of \( \alpha \) laths in the transformed \( \beta \). When \( \alpha \) laths are thick, \( \alpha \) globules show a Hall-Petch type behavior, where a decrease in their size results in an increase in yield strength. However, when the \( \alpha \) laths in the transformed \( \beta \) region become very thin, then for a fixed volume fraction of globular \( \alpha \), materials become stronger when the transformed \( \beta \) region is more continuous, which happens when the size of \( \alpha \) globules increases, because the number of \( \alpha \) globules in a particular volume decreases with increasing average size at a fixed volume fraction. So, it is postulated that when the \( \alpha \) laths in a transformed \( \beta \) region are very thin, the strength of the material can primarily be attributed to those thin \( \alpha \) laths; however, as the thickness of the \( \alpha \) laths increases, the size of globular \( \alpha \) begins to play a more important role in strengthening the material through the Hall-Petch relation. The actual physical mechanisms behind these phenomena are under the scope of further research. Neural Network modeling has helped recognize and better understand the physical mechanisms behind strengthening of these materials, and can help guide and direct further research into their microstructure-property relationships.
Figure 6.1: Significance of the various input parameters on Yield Strength (β heat-treated samples)

Figure 6.2: Predictions of the Yield Strength from microstructures. (β heat-treated samples)
Figure 6.3: Predictions of the Ultimate Tensile Strength (UTS) from microstructures. (β heat-treated samples)

Figure 6.4: Predictions of the Elongation from microstructures. (β heat-treated samples)
Figure 6.5: Experimental Yield Strength values plotted against Thickness of $\alpha$ laths. For this figure, the values of all other microstructural features are varying as well.

Figure 6.6: Trend plot of yield strength variation with thickness of $\alpha$ lath while other microstructural features have been kept constant.
Figure 6.7: Trend plot of yield strength variation with colony size factor (CSF) while other microstructural features have been kept constant.

Figure 6.8: Trend plot of yield strength variation with volume fraction of total $\alpha$ while other microstructural features have been kept constant.
Figure 6.9: Trend plot of yield strength variation with prior $\beta$ grain factor (PBGF) while other microstructural features have been kept constant. NOTE: Larger the PBGF is smaller the prior $\beta$ grain size is.
Figure 6.10: The smaller prior $\beta$ grain contains fully colony microstructure, but the larger prior $\beta$ grain has a basketweave region at the grain interior. (Prior $\beta$ grain boundaries have been depicted by hand-drawn white line for better clarity.)
Figure 11: Trend of Yield Strength (YS) variation with Prior $\beta$ grain factor (PBGF) for two separate databases

Figure 12: Trend of YS variation with Prior $\beta$ grain factor when the volume fraction of basketweave microstructure is an additional input of the neural network
Figure 6.13: Variation in elongation with thickness of $\alpha$ lath while other microstructural features have been kept constant at mean values in their range.

Figure 6.14: Variation in elongation with colony size factor (CSF) while other microstructural features have been kept constant at mean values in their range.
Figure 6.15: Variation in elongation with volume fraction of total $\alpha$ while other microstructural features have been kept constant at mean values in their range.

Figure 6.16: Variation in elongation with prior $\beta$ grain factor (PBGF) while other microstructural features have been kept constant at mean values in their range.
Figure 6.17: Performance of the microstructure based neural network model on β-annealed samples. Input variables are volume fraction of colony, α lath thickness, prior β grain factor and colony size factor. Here, the predicted yield strength (YS) has been plotted against the experimental YS.

Figure 6.18: Performance of the microstructure based neural network model on β-annealed samples. Input variables are volume fraction of colony, α lath thickness, prior β grain factor and colony size factor. Here Predicted ultimate tensile strength (UTS) has been plotted against the experimental UTS.
Figure 6.19: Performance of the microstructure based neural network model on β-annealed samples. Input variables are volume fraction of colony, α lath thickness, prior β grain factor and colony size factor. Here Predicted elongation has been plotted against the experimental elongation.
<table>
<thead>
<tr>
<th>Enter Values</th>
<th>VF of Colony</th>
<th>CSF (µm)</th>
<th>PBGF (mm²/mm³)</th>
<th>Lath Thickness (µm)</th>
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</thead>
<tbody>
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<td>0.97</td>
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</tbody>
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| Best Guess YS value (ksi) | 128.79 |

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**DO NOT CHANGE ANY VALUE BELOW THIS LINE**

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<th>Model1 (m1)</th>
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<th>m1w12_1</th>
<th>m1_w13_1</th>
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<th>VF of Colony</th>
<th>CSF (µm)</th>
<th>PBGF (mm²/mm³)</th>
<th>Lath Thickness</th>
<th>YS (ksi)</th>
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<td>31.472</td>
<td>0.502</td>
<td>0.157</td>
</tr>
<tr>
<td>max.</td>
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<td>433.654</td>
<td>1.398</td>
<td>0.788</td>
</tr>
<tr>
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<td>-0.4201158</td>
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<td>-0.13391</td>
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| m1_a1        | 0.697143709 |
| m1_a2        | -0.646195832 |
| m1_a3        | -1.136461113 |
| m1_a4        | -0.601463387 |

| m1_h1        | 0.602551646 |
| m1_h2        | -0.569103456 |
| m1_h3        | -0.813219006 |
| m1_h4        | -0.538090062 |

Figure 6.20 (Continued)

Figure 6.20: Spread-Sheet version of the end-user tool for prediction for yield strength of β-annealed samples. The rest of the values of model parameters are on the next page.
Figure 6.20 (Continued)

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<tr>
<th>Parameter</th>
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Values of the rest of the model parameters

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<td>CSF (mm²/mm³)</td>
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Best Guess UTS value (ksi) 142.51

---DO NOT CHANGE ANY VALUE BELOW THIS LINE---

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<th>m1_w14_1</th>
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</tbody>
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<table>
<thead>
<tr>
<th>VF of Colony</th>
<th>CSF (µm)</th>
<th>PBGF (mm²/mm³)</th>
<th>Lath Thickness (µm)</th>
<th>UTS (ksi)</th>
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<tbody>
<tr>
<td>min.</td>
<td>0.048</td>
<td>31.472</td>
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<td>0.157</td>
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<td>max.</td>
<td>1</td>
<td>433.654</td>
<td>1.398</td>
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<td>normalized</td>
<td>-0.353991597</td>
<td>-0.4201158</td>
<td>0.022321</td>
<td>-0.13391</td>
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| m1_a1        | 1.189955405 |
| m1_a2        | 1.857010817 |
| m1_a3        | -0.557896333 |
| m1_a4        | -1.335821175 |
| m1_h1        | 0.830565037 |
| m1_h2        | 0.952401846 |
| m1_h3        | -0.506414931 |
| m1_h4        | -0.870664882 |

Figure 6.21 (Continued)

Figure 6.21: Spread-Sheet version of the end-user tool of prediction for ultimate tensile strength (UTS) of β-annealed samples. Complete list of model parameters are on the next page.
Figure 6.21 (Continued)

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**Complete list of model parameters**

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<th>m1_w13_1</th>
<th>m1_w14_1</th>
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</thead>
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<td>-5.98204</td>
<td>0.060483</td>
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<table>
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<tr>
<td>Enter Values</td>
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<td>CSF (µm)</td>
<td>PBGF (mm²/mm³)</td>
<td>Lath Thickness (µm)</td>
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Best Guess Elongation value (%) 6.19

-------------------DO NOT CHANGE ANY VALUE BELOW THIS LINE-----------------

Model 1 (m1) m1_01_1 m1w11_1 m1w12_1 m1_w13_1 m1_w14_1 m1_02_1
10^6-4-1' -1.41719 -2.00372 2.93813 15.1365 4.69256 -1.20742

Model 2 (m2) m2_01_1 m2w11_1 m2w12_1 m2_w13_1 m2_w14_1 m2_02_1
10^4-3-5' -2.37773 0.268468 -4.00624 6.73071 1.18695 -2.26774

Figure 6.22 (Continued)

Figure 6.22: Spreadsheet version of the end-user tool for prediction of elongation of the β-annealed samples. Complete list of the model parameters are on the next page.
Figure 6.22 (Continued)

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Complete list of the model parameters

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165
Figure 6.23: Snapshot of the design tool for yield strength of β annealed Ti-6Al-4V

\[
\text{Yield Strength (ksi) = 121.6}
\]

Figure 6.24: Snapshot of the design tool for ultimate tensile strength of β annealed Ti-6Al-4V

\[
\text{Ultimate Tensile Strength (ksi) = 123.}
\]
Figure 6.25: Snapshot of the design tool for elongation of $\beta$ annealed Ti-6Al-4V

Figure 6.26: Performance of the neural network for prediction of the Yield Strength (YS) prediction based on processing parameters

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Figure 6.27: Performance of the neural network for Ultimate Tensile Strength (UTS) prediction based on the processing parameters. Predicted vs experimental UTS is plotted.

Figure 6.28: Performance of the neural network for Elongation prediction based on the processing parameters
Figure 6.29: Performance of the neural network for Reduction of Area prediction based on the processing parameters. Predicted vs Experimental Reduction of Area is plotted here.

Figure 6.30: Performance of the neural network for Fracture Toughness prediction based on processing parameters.
Figure 6.31: a) Microstructure of a low yield strength $\alpha+\beta$ forged sample; b) Microstructure of a high yield strength $\alpha+\beta$ forged sample
Figure 6.32: Performance of neural network for predicting the YS from the microstructures of $\alpha+\beta$ forged bimodal structures.
Figure 6.33: Trend of yield strength (YS) variations with microstructural features in case of bimodal microstructure. Note: Increasing trend of YS with increasing size of globular $\alpha$ when $\alpha$ lath thickness in transformed $\beta$ is set constant at small values.

Yield Strength (ksi) = 137.3

Figure 6.34: Trend of yield strength (YS) variations with microstructural features in case of bimodal microstructure. Note: Decreasing trend of YS with increasing size of globular $\alpha$ when $\alpha$ lath thickness in transformed $\beta$ is set constant at larger values.

Yield Strength (ksi) = 122.2
CHAPTER 7

MODELING OF FRACTURE TOUGHNESS IN Ti-6Al-4V

7.1 Fracture Toughness Modeling and Fractography Study of β heat-treated Ti-6Al-4V:

7.1.1 Neural Network Modeling of Fracture Toughness for β heat-treateded Ti-6Al-4V Samples: The fracture toughness, $K_{IC}$ is an important property in titanium alloys as it controls the size of a fracture-critical component. Improvement in the $K_{IC}$ of a material provides a better design capability with significant decrease in the weight of the components [106]. So, it is important to identify the parameters that influence $K_{IC}$. In existing literature, many factors have been suggested as those controlling $K_{IC}$; [106] they are texture, modulus, microstructure and environment. Among these factors; microstructure can be varied in titanium alloys widely by applying different thermomechanical treatments. So, it is of practical importance to build a microstructure based fracture toughness models for titanium alloys.

In the present research, microstructure based fracture toughness models have been developed for β heat-treated Ti-6Al-4V samples. Neural network modeling has been employed as the predictive tool for the fracture toughness models. The neural network modeling efforts, in this case, were evolutionary in the sense that different models for
fracture toughness have been developed by including and later discarding some of the inputs and in some step dividing the database into β annealed and β processed samples and remodeling on only the β annealed samples. These modeling efforts will be discussed in this section chronologically as they were developed during the progress in research. Subsequently, the results for the latest Toughness model will be discussed.

7.1.1.1 First approach towards Toughness modeling: At the beginning of the toughness model development work, there were 86 β heat treated samples provided by industry through the Metals Affordability Initiative (MAI) program. The first step was to identify the important microstructural features. This has been discussed in the literature review and database development chapters. From the existing literature findings and from industry experience, five microstructural features were selected initially. They were the volume fraction of total α, thickness of α laths, colony size factor, prior β grain factor and grain boundary α width. These were used as inputs for the network, based on which fracture toughness (KIC) was to be predicted. The statistics for the neural network model that was developed are presented in table 7.1.

For training the neural network, 16 samples had been randomly separated out of the 86 data out as testing set (used for optimizing the model architecture along with initial values of the parameter vector of the network), and the remaining 70 samples were used for training the network (optimizing the parameter vector by minimizing the sum square error). The general training procedure has been described in detail in the Neural Network chapter. As described earlier, optimizing the network architecture is a major part of the

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neural network training. The number of nodes in the hidden layer, initial values of the weight parameters and initial width of the Gaussians corresponding to the weight vector describe network architecture. Initial values of the weight vector in a particular architecture are assigned by a random number generator, called Seed. So, the values of seed, number of hidden nodes and initial Gaussian width form a particular architecture of a neural network; for this database the best fit model architecture was found to be for the following values of those parameters: 100, 2 and 0.5, respectively.

7.1.1.2 Second stage of Toughness modeling: In the next level of toughness modeling, the volume fraction of total α was taken out and the same database was retrained with the inputs α lath thickness, colony size factor, prior β grain factor and width of grain boundary α. The volume fraction of total α was taken out because of the industry partners’ opposition to include this variable as an input; they cited that in a particular alloy, for example Ti-6Al-4V in this case, the volume fraction of total α should not vary over an appreciable range. By training the network, the best fit model architecture was found to be for the following values of seed, number of hidden nodes and initial Gaussian width as 10^6, 5 and 1.0 respectively.

7.1.1.3 Third stage of Toughness modeling: In the next stage, a new microstructural feature, namely the volume fraction of basketweave, has been included as another input. As mentioned in the earlier section, through the tensile property modeling this new microstructural feature has been identified as an influential variable for
mechanical property-model development. The training gave the best fit on the data for a combination of four different architectures of network. As mentioned earlier, if the values of seed, number of hidden nodes and initial Gaussian width are written in the order; those four models in the committee model can be written as 10, 4, 0.5 for the first model, 500, 2, 3.0 for the second model, 10, 4, 0.01 for the third model and 10^6, 5, 1.0 for the fourth model. This network predicted the fracture toughness values from the microstructural features of 16 test samples reasonably well, as can be seen in figure 7.1.

7.1.1.4 New Findings from previous models ---before going to the next stage of the modeling effort:

At this point, we reflected upon our previous modeling efforts and new findings in terms of identification and definition of microstructural input parameters, characterization techniques for their measurements and the processing history of the samples in database were discussed. It was decided that the microstructural features which would be used for fracture toughness prediction of colony/ basketweave microstructure are $\alpha$ lath thickness, colony size factor, prior $\beta$ grain factor, width of grain boundary $\alpha$, and volume fraction of basketweave.

In terms of characterization techniques, few aspects needed attention at this point. The volume fraction of basketweave region in the samples had to be measured; for this, the basketweave region had to be defined. It has been defined as a cluster of different variants in a region, keeping note that within each variant the number of $\alpha$ laths should not be more than three. The next consideration dealt with the measurement of colony size
factor. It was decided that the colony size would be measured only in the colony region, avoiding the basketweave region. So, Colony sizes were re-measured in each sample accordingly. Also, the prior $\beta$ grain size measurement has been redone on huge stitched images making sure that in each image there are at least 6 grains.

In terms of the processing history of the samples in the database, as mentioned earlier, it was recognized that the database contains both $\beta$-annealed and $\beta$-processed samples and was suggested that only $\beta$-annealed samples should be used for the property modeling because for Ti-6Al-4V the $\beta$-anneal treatment is typical for industry.

7.1.1.5 Latest modeling effort towards microstructure based fracture toughness prediction: In view of these decisions, 52 $\beta$-annealed samples were used for remodeling the toughness after the re-measurement of the few microstructural features identified in the previous paragraphs. The ranges of the microstructural features and the fracture toughness of these $\beta$-annealed samples were tabulated and shown in the “Microstructure Characterization & Database Development” chapter. The training gave the best fit on the data for a combination of two different network architectures. As mentioned earlier, the values of seed, number of hidden nodes and initial Gaussian width for those two models in the committee model can be written as 10, 2, 10.0 for the first model and 10, 3, 10.0 for the second model, respectively.

Experimental toughness values in the database have been plotted against each individual microstructural parameter to give a clear idea about the presence and scarcity of the data in the range of the microstructural features (See Figures 7.2 through 7.6).
Prediction has been made on both the training and test samples from the microstructural features using the trained network. This is shown in figure 7.7. Blue dots are predictions on the training set samples, while pink dots are predictions on the test set samples. All the test set samples are seen to fall within +/- error lines, showing a good performance on the test set implying that the trained network’s generalization capability is good. The network has been used not only to give microstructure-based predictions for the fracture toughness of the β-annealed samples, but it also has been used to do some virtual experiments to evaluate the trend of variations of toughness with individual microstructural features while rest of the microstructural features are kept constant. A JAVA-based design tool has been developed where these trend plots of variation of fracture toughness on individual microstructural features can be seen while keeping the values of the rest of the microstructural features constant at any value in their range of variation. Here four snapshot examples of that design tool would be shown at different values of the microstructural features.

Figure 7.8 shows the trend plots when volume fraction of colony microstructure as opposed to basketweave region is set to be 100%. It is seen from the design tool that fracture toughness in fully colony microstructure is maximum when colony size is the largest, prior β grain size is the largest, grain boundary α width is the smallest and α lath thickness is the smallest. The high toughness here, due to large colony size and large prior β grain size, can be attributed to the fact that the energy required for the crack to progress, \( \varepsilon_{\text{path}} \) in the case of large colony size and prior β grain size is greater; this is because the crack has to re-orient itself through a larger angle during its progress each
time it sees a new facet of colony or a prior $\beta$ grain boundary. As a result, the energy of fracture is greater in large colonies and large prior $\beta$ grains. The small width of grain boundary $\alpha$ is making the material tougher; this can be explained in the following way: the $\alpha$ phase is less plastically deformable than the $\beta$ phase. So, the plastic zone ahead of a growing crack tip will be smaller in the $\alpha$ phase, making the crack progress through this phase easier. This makes the grain boundary $\alpha$ layer a good place for crack to grow more quickly. So, a continuous thick layer of $\alpha$ decorating the grain boundary is detrimental in terms of the fracture toughness of a material.

Figure 7.9 shows another example of the trend plots at different value for the volume fraction of colony microstructure. It shows the trend plots when the microstructure is mostly basketweave. It is seen that, when the microstructure is mostly basketweave, the toughness is high when the prior $\beta$ grain size and colony size are both large and the $\alpha$ laths are thin as before. This time, however, high toughness is seen to be at some intermediate value of grain boundary $\alpha$ width. The effect of grain boundary $\alpha$ width in this case is not so great; this might be due to the fact that a crack can grow through the grains more easily in this case because the crack path won’t be so tortuous because the effective colony size is much smaller.

Another interesting observation is that toughness is actually increasing with increasing volume fraction of colony as opposed to basketweave region. This can again be understood by the path term in the fracture energy relationship described in the following section. When the volume fraction of colony microstructure is large, a crack progressing along colony boundaries has to change its direction through a larger angle.
compare to the case where there is mostly basketweave region in the microstructure because in the basketweave region effective colony size is small and crack path tortuosity is low. As a result, less energy is required for fracture in basketweave microstructure, giving a lower value of fracture toughness for basketweave microstructure. This trend of an increase in fracture toughness with increasing volume fraction of colony microstructure is shown in figure 7.8. However, this trend is not always the case, as can be seen in figure 7.10. When the grain boundary is decorated by a wide layer of continuous α phase, the effect (positive trend) of an increase in fracture toughness with an increase in volume fraction of colony decreases. Even this trend becomes slightly negative if the grain boundary α width is very large. This might be due to the change in crack path with a change in grain boundary α width. When the grain boundary α width is very large, a crack prefers to grow along the grain boundary through the α phase, thereby decreasing the effect of volume fraction of colony/ basketweave inside grains. However, when the grain boundary α width is small, the crack prefers to progress along the colony boundaries, increasing the effect of volume fraction of colony vs basketweave.

7.1.2 Fractography (Fracture Surface Analysis) for β annealed Ti-6Al-4V Samples: In the previous section, it is discussed how the fracture toughness can be predicted from microstructural variables in Ti-6Al-4V. Existing literature [106] shows that, in many cases, there are good correlations between the microstructure and fracture topography. So, the fracture topography study is thought to be a useful tool for predicting the relation between microstructure and fracture toughness among the different samples.
Fracture surface topography can help understand the fracture toughness of a sample. The progression of the crack path, its reorientations as it progresses and local crack extension details are qualitatively revealed from the fracture topography; these are indicative of the fracture toughness. In this section, a few fractography results from two samples are presented and analyzed to show the comparative analysis of two extremes in fracture toughness. These are among the samples used to construct the neural network model for $\beta$ annealed Ti-6Al-4V.

Samples designated 02-03 and 21-08 represent two toughness extremes of $\beta$ annealed Ti-6Al-4V. While sample 02-03 has toughness of 108.4 ksi in$^{1/2}$, sample 21-08 has a much lower toughness value of 74.3 ksi in$^{1/2}$. Figure 7.11 shows a fractured sample specimen. In each fracture toughness sample, three distinct zones are seen; namely machine notch, fatigue pre-crack region and unstable fast fracture region. Macroscopically, the fatigue pre-crack growth region can be distinguished from the fast crack growth region by its increased shininess, resulting from the repeated opening and closing of the material under cyclic load. Microscopic fracture topography also shows the clear demarcation between the fatigue pre-crack growth region and unstable fast crack growth region (See figure 7.12 and 7.13). Another distinction between fatigue pre-crack growth region and fast crack growth region is that the fatigue pre-crack growth region has almost no shear lips present along the edge of the sample, while the fast crack growth region shows shear lips at the specimen’s edges. This is due to the fact that, in the fatigue pre-crack growth region, the plastic zone size ($r_p$) ahead of the crack tip is smaller than in the fast crack growth region. This can be understood by the following reasoning. The
plastic zone size, $r_p$ is proportional to $\frac{K^2}{Y^2}$, where $K$ and $Y$ are fracture toughness and yield strength, respectively. During cyclic loading, the material in the plastic zone yields in tension and undergoes reverse yielding in compression during unloading. Thus, the yield strength is effectively doubled (i.e., $Y_{\text{effective}} = 2Y$). Hence, the plastic zone size ($r_p$, here, $r_p = \frac{K^2}{Y_{\text{effective}}^2} = \frac{K^2}{4Y^2}$) in the fatigue pre crack growth region is $\frac{1}{4}$th of that in the fast crack growth region.

Fracture topography images are shown in figures 7.14 through 7.19. These fractographs have been taken in secondary electron mode. Figures 7.14 through 7.16 are fractographs of the high fracture toughness sample 02-03 and figures 7.17 through 7.19 are fractographs of lower fracture toughness sample 21-08.

For a comparative study of the fracture toughness of these samples, at least two factors which influence the energy dissipation during crack extension must be considered. The energy of fracture $\varepsilon_f$ is proportional to the energy dissipated in re-orientation of the crack path during its progress, given by $\varepsilon_{\text{path}}$ and the energy for local crack extension, given by $\varepsilon_{\text{loc.crackext}}$. [107].

$$\varepsilon_f \propto \varepsilon_{\text{path}} \times \varepsilon_{\text{loc.crackext}}.$$ 

Considering the first factor, from the surface roughness/irregularities off the plane in figures 7.15 and 7.16, it is seen that the crack had to reorient itself through large angles during its travel through the material, causing a high value of $\varepsilon_{\text{path}}$ in sample 02-03. In sample 21-08, the fracture surface is not so rough and does not show appreciable off-the-
plane extension of the facets, proving that less energy has to dissipate to re-orient the crack during its progress through the material. Comparing the fractographs of the two samples, it is seen that, while in sample 02-03 secondary cracks are present, no such secondary crack is present in sample 21-08. Secondary cracks are indicative of higher tortuosity of the crack path; a tortuous crack path will leave behind some secondary cracks. Appreciable energy has to be dissipated to form these secondary cracks, causing the value of the first term in the energy relationship, $\varepsilon_{\text{path}}$, appreciably larger in sample 02-03 than that in 21-08.

Figure 7.14 shows elongated flutes in the fractographs of sample 02-03, giving the appearance of serpentine glide or stretch marks. Lots of energy had to be dissipated to make these large hollows. The presence of large scale plasticity in this sample caused a high value of $\varepsilon_{\text{loc.cracked}}$. In contrast, in the fractographs of sample 21-08, no such big hollows are apparent. The average dimple size is much smaller in this sample’s fracture surface. No large local plasticity region is seen. So, we can conclude that much less energy was spent for the local crack extension in this sample, implying a very low value of $\varepsilon_{\text{loc.cracked}}$.

In view of the foregoing evidence, it is argued that values for both terms in the energy equation are larger in sample 02-03; the energy of fracture is much higher in this sample compared to the other sample 21-08. Fractographs taken near the fatigue-fast fracture transition are very effective in giving a comparative idea of the fracture toughness of different samples.
Another interesting point [107] to be noted here in relation to the above mentioned relationship for fracture energy is that the presence of the first term, $\varepsilon_{path}$ and its higher value in $\beta$ processed colony type of microstructure than that in $\alpha+\beta$ forged bimodal microstructure causes the $\beta$ processed Ti-6Al-4V to have a greater fracture toughness ($K_{IC}$) than that of $\alpha+\beta$ forged Ti-6Al-4V, although $\alpha+\beta$ forged samples have higher % elongation values than those of the $\beta$ processed samples. This fact might appear contradictory to someone with experience with steel where % elongation values generally correlate well with fracture toughness and inverse correlations such as shown here are not observed.

7.2 Fracture Toughness Modeling of $\alpha+\beta$ forged Ti-6Al-4V:

Neural network modeling has been developed for the prediction of $\alpha+\beta$ forged Ti-6Al-4V with bimodal microstructure. 34 such samples were obtained from industry through the Metals Affordability Initiative program. The heat treatment schedules have been described in section 4.2.1. Microstructures were characterized to have quantified data of the following four microstructural parameters: volume fraction of total $\alpha$, volume fraction of globular $\alpha$, size of globular $\alpha$ and thickness of $\alpha$ laths in transformed $\beta$. The ranges and standard deviations of all microstructural features along with toughness values in the database have been shown in table 4.5.

A predictive model for the toughness of these $\alpha+\beta$ forged Ti-6Al-4V samples was made using the fuzzy logic neural network tool. All 34 data were trained; rules were
generated using the RuleMaker module by setting the adjective for each variable as 4. Performance of this fuzzy network is seen in figure 7.20, where the predicted toughness has been plotted against the experimental toughness for those 34 samples. These are microstructure-based predictions. Most of the data are seen to fall within +/- 5% error lines.

The trained network was used to get the trend plots for the fracture toughness variation with individual microstructural features while other microstructural features were kept constant at their respective average values shown in table 4.5. Trend plot of toughness variation with volume fraction of total $\alpha$ is shown in figure 7.21. Toughness is seen to decrease with an increase in the volume fraction of total $\alpha$. This can be understood in the following way: because the $\alpha$ phase is stronger than the $\beta$ phase, the plastic zone size in front of the crack tip is smaller in the $\alpha$ phase than in the $\beta$ phase. As a result, a crack can progress more easily through the $\alpha$ phase than in the $\beta$ phase. So, as the volume fraction of total $\alpha$ increases, the fracture toughness of the material decreases. Figure 7.22 shows the trend plot of toughness variation with volume fraction of globular $\alpha$. The toughness decreases with increasing volume fraction of globular $\alpha$. As the transformed $\beta$ regions with colonies of $\alpha$ laths provide a more tortuous path for crack propagation, an increase in this transformed $\beta$ region (hence, a decrease in the volume fraction of globular $\alpha$) causes the fracture toughness of the bimodal microstructure to increase. Figure 7.23 shows the effect of globular $\alpha$ size on the fracture toughness. As the globular $\alpha$ size increases, the fracture toughness of the material increases. This might be
due to two reasons. First, with increasing size of globular $\alpha$, a crack has to travel through a particular globular $\alpha$ for a longer distance. Secondly, if the volume fraction of globular $\alpha$ is fixed, then with an increase in the size of globular $\alpha$, number of globular $\alpha$ decreases and the continuity of transformed $\beta$ region increases, which makes the crack path to be more tortuous; as a result with increase in size of globular $\alpha$ the energy dissipated for the crack to progress (the path term in the fracture energy equation, $\varepsilon_{path}$) increases, thereby increasing the fracture toughness of the material. Figure 7.24 shows the effect of $\alpha$ lath thickness in the transformed $\beta$ region. Here, we see that, similar to $\beta$ annealed colony/basketweave microstructure, fracture toughness is high for thin $\alpha$ laths. Crack growing through a colony of a fixed size will meet more $\alpha/\beta$ interfaces (which give more resistance than the continuous single phase) on its progress path in case when the $\alpha$ laths are thin than the case where $\alpha$ laths are thicker. This might be the reason for fracture toughness of a material to increase with decrease in $\alpha$ lath thickness.
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Table 7.1: Statistics of the various input and output parameters in the initial toughness database for $\beta$ heat-treated samples
Figure 7.1: Predicted Toughness vs Experimental Toughness for β-heat-treated (both β-processed and β-annealed) samples. Prediction is based on the following microstructural features: volume fraction of basketweave, thickness of α lath, colony size factor, grain boundary α width and prior β grain factor.
7.2: Experimental Toughness values plotted against volume fraction of colony (all other microstructural features are varying too)

7.3: Experimental Toughness values plotted against thickness of $\alpha$ laths (all other microstructural features are varying too)
7.4: Experimental Toughness values plotted against colony size factor (all other microstructural features are varying too)

7.5: Experimental Toughness values plotted against width of grain boundary $\alpha$ (all other microstructural features are varying too)
7.6: Experimental Toughness values plotted against prior β grain factor (all other microstructural features are varying too)

Figure 7.7: Prediction of toughness of β-annealed samples based on microstructural features
Figure 7.8: Trend plots of fracture toughness variation with individual microstructural features for β-annealed samples. Note: Here microstructure is mostly colony.

Toughness (ksi.in^{(1/2)}) = 121.6

Figure 7.9: Trend plots of fracture toughness variation with individual microstructural features for β-annealed samples. Note: Here microstructure is mostly basketweave.

Toughness (ksi.in^{(1/2)}) = 114.3
Figure 7.10: Trend plots of fracture toughness variation with individual microstructural features for $\beta$-annealed samples. Note: Toughness increases with increase in volume fraction of colony.

Toughness (ksi.in^{(1/2)}) = 104.9
Figure 7.11: a) Side view of the fracture toughness sample; b) Top view of the fracture toughness sample
Figure 7.12: Transition between Fatigue pre-crack growth region and fast fracture region (Boundary approximately indicated by dotted line)
Figure 7.13: Transition between Fatigue pre-crack growth region and fast fracture region (Boundary approximately indicated by dotted line)
Figure 7.14: Fracture topograph of high-end fracture toughness sample, 02-03. Large serpentine glide / stretch marks
Figure 7.15: Fracture topograph of high-end fracture toughness sample, 02-03. Local Ductility and Secondary Cracks make it pretty tough
Figure 7.16: Fracture topograph of high-end fracture toughness sample, 02-03. Grain boundary facets showing large crack path reorientation angle, which caused higher toughness of the sample
Figure 7.17: Fracture topograph of low-end fracture toughness sample, 21-08. Relatively very small ductile dimple features.
Figure 7.18: Fracture topograph of low-end fracture toughness sample, 21-08. No serpentine feature, local plastic zone is very small.
Figure 7.19: Fracture topograph of low-end fracture toughness sample, 21-08. No secondary crack formation
Figure 7.20: Performance of fuzzy neural network on predicting fracture toughness for \(\alpha+\beta\) processed bimodal microstructure.

Figure 7.21: Trend of toughness variation with volume fraction of total \(\alpha\) in case of bimodal microstructure.
Figure 7.22: Trend of toughness variation with volume fraction of globular $\alpha$ in case of bimodal microstructure.

Figure 7.23: Trend of toughness variation with size of globular $\alpha$ in case of bimodal microstructure.
Figure 7.24: Trend of toughness variation with thickness of $\alpha$ lath in transformed $\beta$ in case of bimodal microstructure
CHAPTER 8

SUMMARY AND CONCLUSIONS

The research work presented in this dissertation has two primary foci:

1) Study of microstructure evolution in $\alpha/\beta$ Ti alloys.

2) Modeling of microstructure-property relationships in $\alpha/\beta$ Ti alloys.

In the first part of this thesis, different aspects of the microstructure evolution with respect to $\beta$ annealing heat treatment in $\alpha/\beta$ Ti alloys has been discussed. The second part of the thesis was focused on the neural network modeling effort towards understanding microstructure-property relationships in these alloys. In this section, the critical findings from this research effort will be summarized.

8.1 Microstructure evolution in $\alpha/\beta$ Ti alloys:

Titanium alloy microstructures are very complex, composed of features spanning across a range of size scales. Two broad heat-treatment schedules have been performed to obtain $\beta$-heat-treated microstructures in $\alpha/\beta$ Ti alloys. They are: the $\beta$-annealing treatment, where the final step of the heat-treatment is cooling down from above the $\beta$ transus temperature, and the $\beta$-processed treatment, where samples are mechanically...
processed above the β-transus temperature followed by an α+β heat-treatment. The microstructure formed as a consequence of the solid-state $\beta \rightarrow \beta + \alpha$ transformation can effectively be separated into two types. These are the colony microstructure (clustering of α laths belonging to the same variant) and the basketweave microstructure (clustering of multiple variants).

In terms of microstructural evolution, the research effort has been directed towards understanding the colony and the basketweave microstructure addressing critical issues regarding their formation. By coupling characterization techniques that span across a range of length scales (e.g., SEM and TEM), together with the attendant crystallographic information (OIM) and 3D characterization of the microstructure, some of these issues have been addressed. Specifically, the following conclusions can be drawn from these studies:

1) The colony microstructure forms on the side of the grain boundary where the prior β grain observes a Burger’s orientation relationship (OR) with the grain boundary α. The α laths in the colony have the same crystallographic variant, which is in turn identical to that of the grain boundary α.

2) The multiple variants of α laths forming the basketweave microstructure are not randomly selected. Two specific variant selection criteria have been commonly observed:
   - α laths sharing a common [1120] direction that lies parallel to the Burgers [111] β direction in the grain and with their basal [0001] poles rotated by 60° to each other
• α laths sharing a common (0001) basal plane with their $<11\bar{2}0>$ directions being rotated by $\sim 10.53^\circ$ about the common [0001] direction such that all variants satisfy the Burgers OR with the β grain.

The variant selection criteria governing the clustering of α variants in the basketweave microstructure is thought to be a consequence of self-accommodation of these variants that results in a minimization of the overall strain energy resulting from the $\beta \rightarrow \alpha$ transformation.

3) Formation of the basketweave microstructure has been studied as functions of under-cooling and prior β grain size. For a smaller under-cooling below the β transus, primarily colony microstructure forms. The tendency of basketweave microstructure formation increases as the under-cooling increases.

4) A model for basketweave microstructure development has been proposed. The primary mechanism for the formation of the basketweave microstructure appears to be by the continued growth (also referred to as ‘shooting’ earlier in this dissertation) of a few α laths into the grain interior from different colonies growing from different sections of the prior β grain boundary. These laths, belonging to different variants, intersect and give the basketweave appearance. As a colony grows from the grain boundary α layer, beyond a certain length progressively fewer laths continue to grow while other laths stop growing. After further growth, even fewer number of laths continue growing, eventually giving rise to a “single laths shooting inside” appearance. This is happening for different colonies, resulting in a basketweave region at
the center of the grains. The truncated growth of certain laths occurs because these laths encounter (intersect) laths of other variants from neighboring colonies. This is why some laths in the same colony grow longer.

5) For smaller grains, the probability of truncation of laths due to intersections with other variants prior to complete transformation of the β grain is rather small. Therefore, smaller grains typically exhibit a fully colony microstructure

8.2 Modeling of microstructure-property relationships in α/β Ti alloys:

Since α/β Ti alloys exhibit a rather complex multi-scale microstructure, and these microstructural features are closely interdependent, it is very difficult to develop phenomenological models for their microstructure-property relationships. Currently, only a qualitative understanding of microstructure-property relationships in these alloys has been proposed in the literature (by G.Lütjering [21]).

Due to the complexity of the problem, rules-based and neural networks approaches have been employed in the present research. Neural network models allow for a quantitative prediction of the properties from the microstructural input parameters. This is perhaps the first attempt to quantitatively predict the values of various mechanical properties of α/β Ti alloys based on the microstructure. A critical summary of the models and the predictions afforded by these models is discussed below:

8.2.1 β-heat-treated microstructure: Neural networks models have been developed for predicting the tensile properties (YS, UTS and elongation) and the fracture
toughness from the microstructural parameters in the case of the colony/ basketweave microstructure developed by β-heat-treatment in Ti-6Al-4V.

1) Inputs, Outputs and Predictive capability: Microstructural input parameters, based on which predictive models for tensile properties have been developed, are the thickness of the α laths, colony size factor, volume fraction of colony/basketweave and prior β grain factor. For the fracture toughness model, grain boundary α width was an additional input parameter. 52 samples were in each property- microstructure database. In each case, around 2/3rd of the database has been used for training the neural network (optimizing the weight parameters associated with various connections between nodes for a particular model architecture) and remaining 1/3rd of the database has been used as a test set for selecting the best model architecture. Predictions of the YS, the UTS and the fracture toughness on the test set were within +/- 3 % error. However, predictive performance on elongation was not as good; this might be because in these models, the elongation at failure (which is a parameter characteristic of the unstable plastic deformation zone of the stress-strain diagram) has been modeled based on the microstructure of the undeformed material (which has not been deformed plastically in an unstable way, i.e., the microstructure before necking).

2) Influence of Individual Microstructural Parameters on properties: Neural networks allow for virtual experiments, via which the effects of individual microstructural features have been examined. The concept of a virtual
experiment is to see the effect of a specific microstructural feature by varying the values of only that microstructural feature while keeping the values of the rest of the microstructural features constant. YS and UTS have been seen to increase with a decrease in the size scale of the colonies, $\alpha$-lath thickness and prior $\beta$ grains. Colony size is thought to be the effective slip length in available literature. Thus, it follows that decreasing the colony size should increase the YS and UTS because of the decrease in dislocation pile up length. The argument has been that, in a single colony, the $\alpha/\beta$ interfaces provide very little resistance to slip transfer. However, the pronounced trend of an increase in YS with decreasing $\alpha$ lath thickness shown in this work suggests that the $\alpha/\beta$ interfaces possibly act as major barriers to slip. Two possible causes for this, either the strength of the $\alpha/\beta$ interfaces or the constrained deformation behavior of the $\beta$ ribs between the $\alpha$ laths, are promising areas for further research. In the initial tensile property model, where % colony/basketweave microstructure had not been used as an input, a decrease in the prior $\beta$ grain size was predicted to decrease YS and UTS, contradicting Hall-Petch behavior. Careful characterization of the microstructures with large and small prior $\beta$ grains revealed the importance of % colony/basketweave microstructure. In later models, when % colony/basketweave has been used as an additional input parameter, the effect of prior $\beta$ grain size could be separated out from the % colony/basketweave resulting in a change in the
trend of strength variation with prior $\beta$ grain size from increasing to decreasing.

The microstructure-based fracture toughness model shows that the fracture toughness becomes high when the colony size and the prior $\beta$ grain size are large, grain boundary $\alpha$ width is small and $\alpha$ lath thickness is small. In case of larger colonies and prior $\beta$ grains, the crack has to re-orient itself through a larger angle each time it sees a new colony facet or a prior $\beta$ grain boundary during its progress through the colony boundary and/or the prior $\beta$ grain boundary, requiring more energy for the crack to progress. A larger grain boundary $\alpha$ width appears to be detrimental to the fracture toughness as the plastic zone ahead of a growing crack tip is smaller in the grain boundary $\alpha$ layer, making the crack’s progress easier. It has been also observed that the fracture toughness increases with increasing volume fraction of colony as opposed to basketweave region. This might be because in the basketweave region, the effective colony size is small and crack path tortuosity is low; as a result, less energy is required for fracture in the basketweave microstructure, giving a lower value of fracture toughness. However, this effect of $\%$ colony/basketweave on the fracture toughness is dependent on the width of grain boundary $\alpha$. This is possibly due to the change in crack path with a change in grain boundary $\alpha$ width. When the grain boundary $\alpha$ width is very large, a crack prefers to grow along the grain boundary through the $\alpha$ phase, thereby
decreasing the effect of volume fraction of colony/basketweave inside grains on the fracture toughness. However, when the grain boundary $\alpha$ width is small, the crack prefers to progress along the colony boundaries in a trans-granular fashion, increasing the effect of volume fraction of colony vs basketweave.

8.2.2 $\alpha+\beta$-forged microstructure: Neural networks models have been developed for predicting the tensile properties (YS, UTS and elongation) and the fracture toughness from the microstructural parameters in the case of the bimodal microstructure developed by $\alpha+\beta$-processing of Ti-6Al-4V.

1) Inputs, Outputs and Predictive capability: The microstructural input parameters, used to develop predictive models for the tensile properties and the fracture toughness are volume fraction of total $\alpha$, volume fraction of globular $\alpha$, $\alpha$ lath thickness in transformed $\beta$ and size of globular $\alpha$. There were microstructure and property values for 135 odd samples. As in the case of the $\beta$-heat-treated samples, 2/3rd of the dataset has been used as a training set and the remaining 1/3rd has been used as a test set. The predictive capability for the test set has been found to be within +/- 5 %.

For fracture toughness prediction, 34 samples’ data were used to model using the fuzzy logic method and commercially available software, CubiCalc. All data were used for training because the dataset was small.
2) *Influence of individual microstructural parameters on properties:* For the bimodal microstructure, a low volume fraction of globular $\alpha$ and thin $\alpha$ laths in transformed $\beta$ region was shown to produce a high yield strength material. An interesting observation was that the trend for yield strength variation with the size of globular $\alpha$ changes from increasing to decreasing as the thickness of $\alpha$ laths in transformed $\beta$ is kept constant at larger values (thick $\alpha$ laths) instead of small values (thin $\alpha$ laths). This might be due to a change in strengthening mechanism accompanied by a change in the thickness of $\alpha$ laths in the transformed $\beta$. When $\alpha$ laths are thick, $\alpha$ globules show a Hall-Petch type behavior, where a decrease in their size results in an increase in yield strength. However, when the $\alpha$ laths in the transformed $\beta$ region become very thin, for a fixed volume fraction of globular $\alpha$ the materials become stronger when the transformed $\beta$ region is more continuous, which happens when the size of the $\alpha$ globules increases, because the number of $\alpha$ globules in a particular volume decreases with increasing average size at a fixed volume fraction. So, it is postulated that when the $\alpha$ laths in a transformed $\beta$ region are very thin, the strength of the material can primarily be attributed to those thin $\alpha$ laths; however, as the thickness of the $\alpha$ laths increases, the size of globular $\alpha$ begins to play a more important role in strengthening the material through the Hall-Petch relation.
From the fracture toughness model, it has been seen that the fracture toughness in the bimodal microstructure increases with a decrease in the volume fraction of total $\alpha$. This is because the $\alpha$ phase is stronger than the $\beta$ phase, and the plastic zone size in front of the crack tip is smaller in the $\alpha$ phase than in the $\beta$ phase. As a result, a crack can progress more easily through the $\alpha$ phase than in the $\beta$ phase. So, as the volume fraction of total $\alpha$ increases, the fracture toughness of the material decreases. In addition, as the size of the globular $\alpha$ increases, the fracture toughness of the material increases. Two reasons have been proposed. First, with an increasing size of globular $\alpha$, a crack has to travel through a particular globular $\alpha$ for a longer distance. Secondly, if the volume fraction of globular $\alpha$ is fixed, then with an increase in the size of globular $\alpha$, number of globular $\alpha$ decreases and the continuity of the transformed $\beta$ region increases, which makes the crack path more tortuous; as a result, with an increase in the size of globular $\alpha$, the energy dissipated for the crack to progress (the path term in the fracture energy equation, $\epsilon_{\text{path}}$) increases, thereby increasing the fracture toughness of the material.

In summary, this dissertation addressed the issues related to microstructure evolution and the microstructure-property relationships in $\alpha/\beta$ Ti alloys. Coupling of multi-scale characterization techniques (Optical Microscopy, SEM, TEM), three-dimensional characterization by FIB, and orientation characterization using OIM helped
to address various issues related specifically to the colony and the basketweave microstructure development. A model has been proposed for the basketweave microstructure formation that could be useful for future Phase Field modeling. Quantitative predictive models have been developed for the mechanical properties in $\alpha/\beta$ Ti alloys based on their microstructures. The complexity of the microstructure in $\alpha/\beta$ Ti alloys in terms of the microstructural features, which not only vary over a wide range of length scales but also are interdependent, makes the task of developing a predictive model for properties based on microstructure very difficult. Using the artificial intelligence capability of the neural network modeling we have been able to successfully predict various mechanical properties of $\alpha/\beta$ Ti alloys from their microstructures. The influences of individual microstructural features have been extracted from the trained neural networks through virtual experiments. It is believed that the information gained from this work will prove to be excellent guidelines for developing mechanistic models for property predictions in $\alpha/\beta$ Ti alloys.

8.3 Unresolved issues to be addressed in future work:

8.3.1 Issues related to microstructure characterization and property modeling:

1) Features that have not been measured, but are probably impacting properties:
   a) volume fraction, size scale and aspect ratio of secondary $\alpha$.
   b) Local oxygen content in the phases
   c) Composition of individual phases-(elemental partitioning)
d) Constraint of $\beta$ – width of $\beta$ laths (possibly containing the secondary $\alpha$ laths)

e) Real, total volume fraction of $\alpha$ (including secondary $\alpha$)

f) Texture

g) In Bimodal microstructure: % colony and basketweave in transformed $\beta$ region.

2) In the bimodal microstructure, impingement of globular $\alpha$ raises the issue of measuring true size of globular $\alpha$.

3) Change in contrast within the same globular precipitate - possibly caused by changes in orientation which has been ignored.

8.3.2 Issues related to microstructure evolution:

1) What is the composition profile ahead of the perturbation (at the very initial stage of slide-plate formation from the grain boundary), and how does this affect further growth of the $\alpha$ lath?

2) Are the $\alpha$ side plates from the grain boundary $\alpha$ continuation of growth of the perturbations on the grain boundary $\alpha$, or due to a sympathetic nucleation of $\alpha$ near the grain boundary?

3) A more detailed study will be required to determine the grain boundary $\alpha$ variant selection criteria, specifically whether one or multiple variants of $\alpha$ are precipitated on the grain boundary.
4) Exact morphology of the growing $\alpha$ laths.

5) When colonies of different variants grow from different parts of the grain boundary and intersect each other, which variant grows further and which variant stops?

6) In the present research, no evidence of homogeneous nucleation has been apparent for the basketweave microstructure development. However, can some experiments be designed to look specifically into the aspects of homogeneous nucleation during basketweave microstructure formation?

7) Detailed study will be required to better understand the influence of the alloy composition and thermal treatment on the morphology of the laths.
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