3.24 Final Project:
Structure and Properties of Titanium and its Alloys

1   Introduction

Titanium has found widespread use for a number of industries in the past 50 years. The metal's corrosion resistance, high specific strength, relatively low density, and manufacturability make it a popular material for a number of applications [1]. Titanium's presence in the aerospace industry is especially prevalent, given the demand for strong, light-weight components required for air- and spacecraft.

Pure titanium, as well as its alloys, has different allotropes with unique crystal structures. These different alloys and crystal structures lead to different material properties, which have important implications for titanium material selection and use. This paper will provide an overview of titanium, its structures, and how those structures impact bulk material properties. There will be a specific discussion on the Ti-6Al-4V alloy, and how its structure and properties compare to those of pure titanium and of its constituent elements.

2   Structure of Titanium

2.1   Pure Titanium

Pure titanium has two crystal structures, and exhibits a crystallographic transformation at 882°C [2]. Below this temperature, titanium has a hexagonal close packed structure, known as the alpha phase of titanium. Above this temperature, titanium has a body centered cubic structure, known as the beta phase of titanium, until its melting point at 1670 °C. A depiction of the alpha and beta phases of titanium is shown in Figure 1.
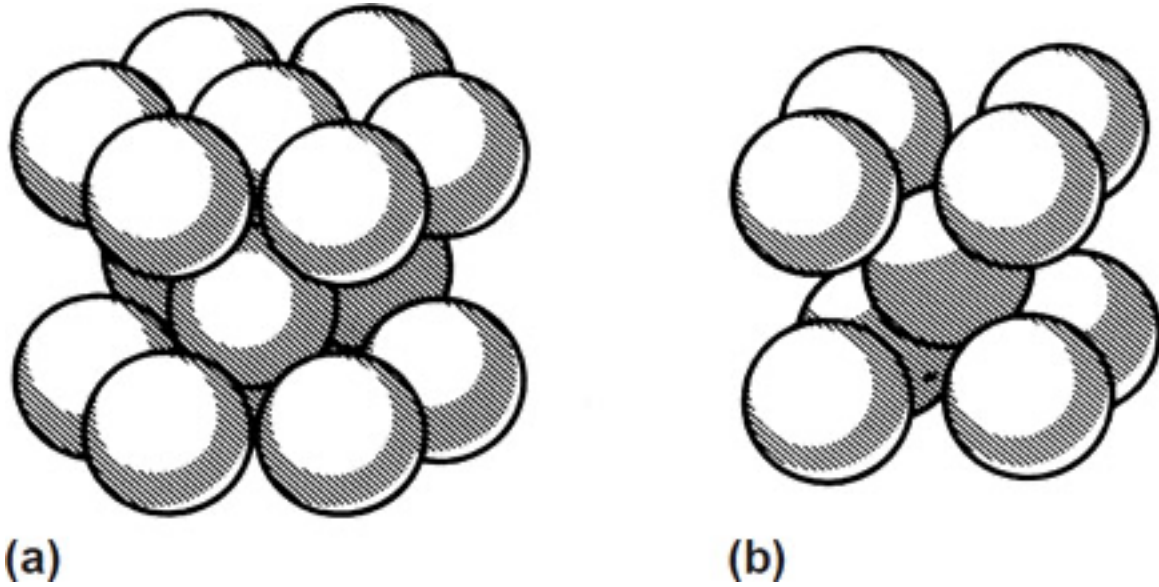
Figure 1 - Depictions of the structures of the alpha (left) and beta (right) phases of titanium. Reprinted from [3].

2.1.1   Slip planes

The atomic arrangements of alpha and beta phase titanium lead to a number of densely packed planes in their structures, as shown in Figure 2. These densely packed planes often become slip planes in the larger crystal. The alpha phase has 3 slip systems and a minimum slip path of $1 \cdot (lattice\ parameter)$, and the beta phase has 12 slip systems and a minimum slip path of $0.87 \cdot (lattice\ parameter)$ [1]. The differences in the number of slip systems and minimum slip path have an important effect on a number properties of the bulk material, discussed further in Section 3 [1] [4].
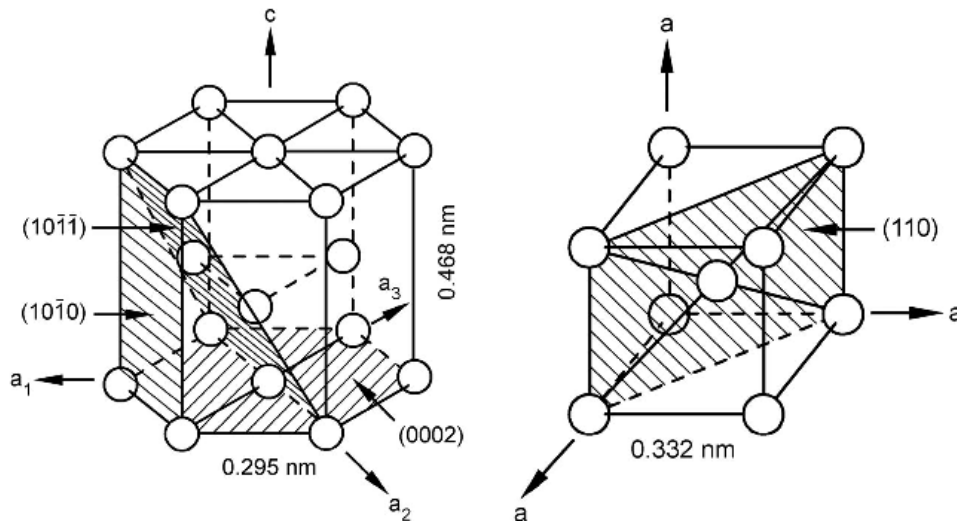

Figure 2 - Densely packed possible slip planes for alpha (left) and beta (right) phase titanium. Reprinted from [4].

2.1.2   Diffusion rate

The different packing densities of the alpha and beta phases of titanium create large differences in the diffusion rates for each phase. Because the alpha phase is more densely packed than the beta phase, diffusion rates for the alpha phase are an order of magnitude less than for the beta phase [1]. These differences in diffusion rate impact several of the bulk material properties, and will be discussed further in Section 3.

2.2   Titanium alloys

Titanium is a transition metal with four valence electrons, and can therefore form solid solutions with several compatible alloying elements. The alloying elements modify the original titanium crystal structure with interstitial or substitutional atoms to form the titanium alloy [2]. An example of atomic substitution for both alpha- and beta-phase titanium is given in Figure 3.
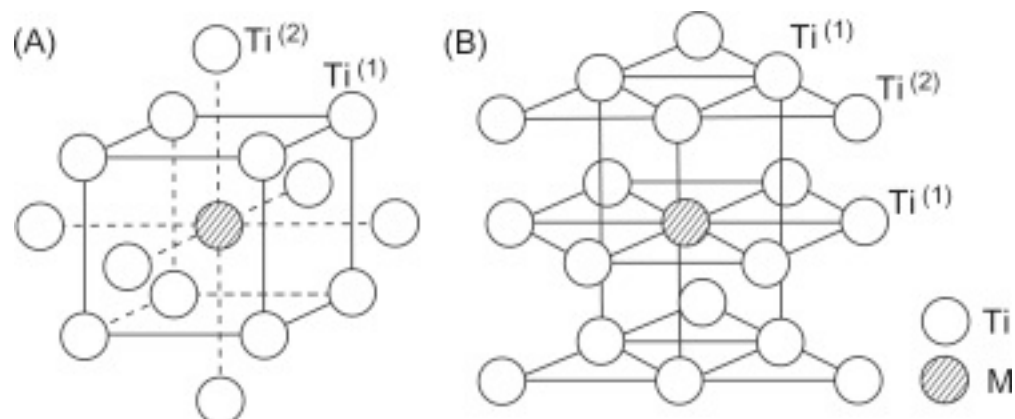

Figure 3 – Depiction of atomic substitution of modifying alloying element (M) for alpha (right) and beta (left) phase titanium. Reprinted from [5].

2.2.1   Effect of Alloying Elements on Local Lattice Stress Field

When substitutional or interstitial elements are introduced into a crystal lattice, they distort the lattice around them and create a local stress field, as depicted in Figure 4 [6] [7]. These stress fields can interact with dislocations within a crystal, impeding their motion and essentially pinning the dislocations in place. This dislocation pinning affects several material properties, including strength and ductility, and will be discussed further in Section 3.
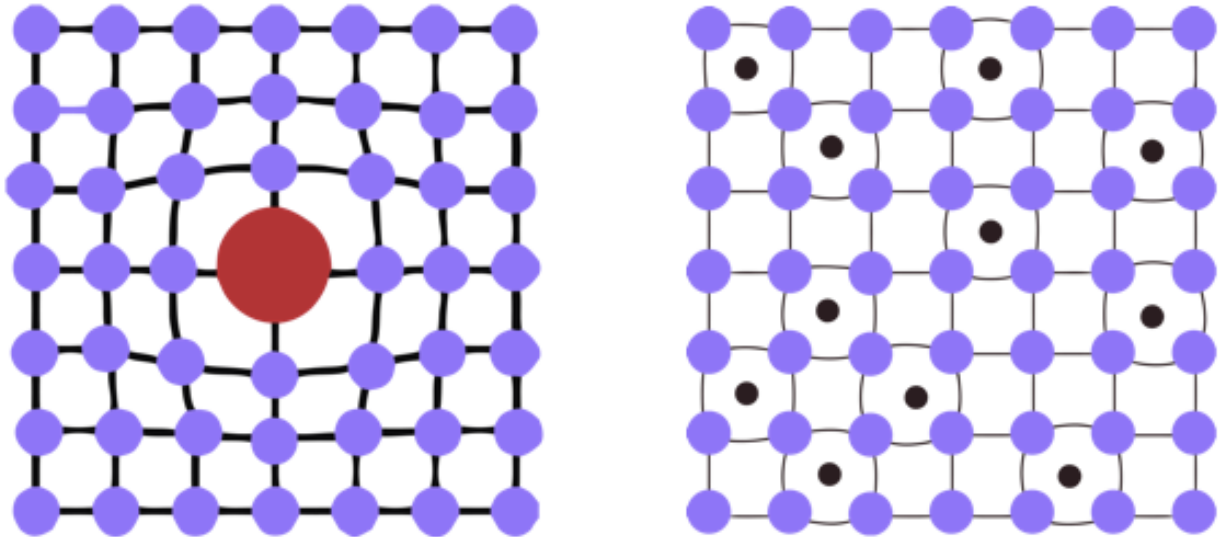
Figure 4 - Depiction of lattice stress field distortion due to substitutional (left) and interstitial (right) solute in lattice. Reprinted from [8].

2.2.2   Classification of Titanium Alloys

Titanium alloys can be classified broadly into three categories depending on their crystal structure [1]:

- Alpha alloys, which maintain the hexagonal close packed structure of the alpha phase of pure titanium.
- Beta alloys, which maintain the body centered cubic structure of the beta phase of pure titanium.
- Alpha+beta alloys, which consist of a two-phase combination of the alpha and beta phases and can have varying microstructure, discussed further in Section 2.2.4.

The addition of alloying elements to titanium can help to stabilize a class of titanium alloys to achieve desired material properties, and is described in the following subsection.

2.2.3   Classification of Alloying Elements

Different alloying elements have different effects on the transformation temperature and properties of titanium alloys. Alloying elements for titanium can be classified into three categories [1]:

- Alpha stabilizers, which extend the alpha-phase field to higher temperatures with the addition of the element.

- Beta stabilizers, which extend the beta-phase field to lower temperatures with the addition of the element; beta stabilizers can be further classified into eutectoid stabilizers, which can nucleate intermetallic compounds in the alloy, and isomorphous stabilizers, which do not.
- Neutral, which have a relatively small effect on the phase transformation temperature of the alloy.

The effects of the different classes of alloying elements on the phase transformation of a binary titanium alloy, as well as some example alloying elements from each class, are shown in Figure 5. Titanium alloys can be made with more than one alloying element as well, from combinations of the above categories. Ternary titanium alloys, containing both an alpha and beta stabilizer, are common. The addition of both an alpha and beta stabilizer can help to broaden the alpha+beta phase, as shown in Figure 6 [9]. Alpha+beta phase titanium will be discussed further in Section 2.2.4. The most widely used titanium alloy, Ti-6Al-4V, is an alpha+beta alloy containing both an alpha and beta stabilizer, and is discussed further in Section 4.
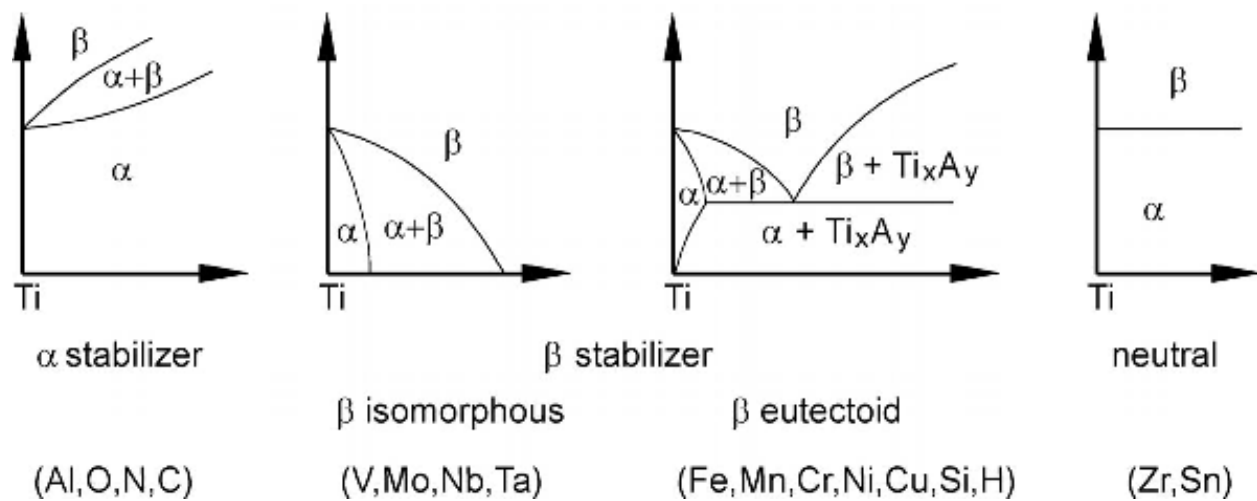

Figure 5 - Alloying elements and their effects on the phase transition of binary titanium alloy. Reprinted from [4].
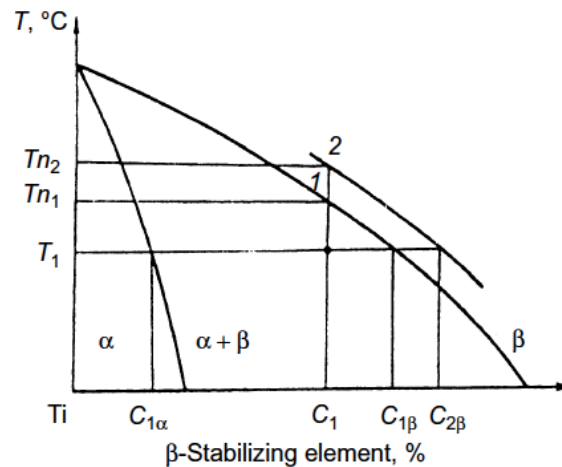
Figure 6 - For a titanium alloy with a beta stabilizer, the further addition of an alpha stabilizer will increase the $\beta \leftrightarrow \alpha + \beta$ transus temperature. For instance, this might change the $\beta \leftrightarrow \alpha + \beta$ phase transition boundary from curve 1 to curve 2 as shown. Reprinted from [9].

2.2.4   Alpha+Beta Alloys

The addition of alloying elements into titanium allows the formation of a new, two-phase alpha+beta structure, which does not exist for pure titanium. Alpha+beta phase alloys can take on a number of different microstructures, depending on the mechanical processing and temperature treatment of the material. The microstructure can be described by the arrangement of the alpha and beta phases, as well as the sizes of those phases. The main phase arrangements of the alpha+beta microstructure are fully lamellar, fully equiaxed, and bi-modal colony arrangements, and will be described further in the following subsections [1] [4] [10].

2.2.4.1   Fully lamellar arrangement

In the fully lamellar structure, alpha-phase lamellae colonies of varying orientation form within larger beta-phase grains, as shown in Figure 7b [10]. The lamellae form when titanium alloy is recrystallized in the beta-phase and then cooled below the β-transus temperature. The cooling rate has a significant effect on the structure of the alpha lamellae, with faster cooling rates yielding thinner lamellae and smaller lamellar colonies within the alloy [4].

2.2.4.2   Fully equiaxed arrangement

The fully equiaxed arrangement consists of globular alpha-phase colonies within a beta-phase matrix, as shown in Figure 7a [10]. After fully lamellar alloy is worked at a lower temperature within the alpha+beta region of the phase field, it is then recrystallized at a higher temperature within the

alpha+beta region (but still below the β-transus temperature) [4]. If the cooling rate from the recrystallization step is slow enough, globular alpha-phase colonies will form, with beta-phase volumes forming at the nodes between alpha colonies. The thickness of the lamellae during the working step effects the size of the alpha globules after recrystallization, with thicker lamellae leading to larger alpha colony size in the fully equiaxed arrangement [4].

2.2.4.3   Bimodal arrangement

In the bimodal arrangement, equiaxed alpha-phase globules exist within a lamellar alpha+beta matrix, as shown in Figure 7c [4]. A bimodal arrangement is formed similarly to the fully equiaxed arrangement, except with either 1) a faster cooling rate after the recrystallization step so that all the alpha-phase globules do not have time to form, or 2) a lower recrystallization temperature such that some alpha globules can form directly from the alpha lamellae [4].
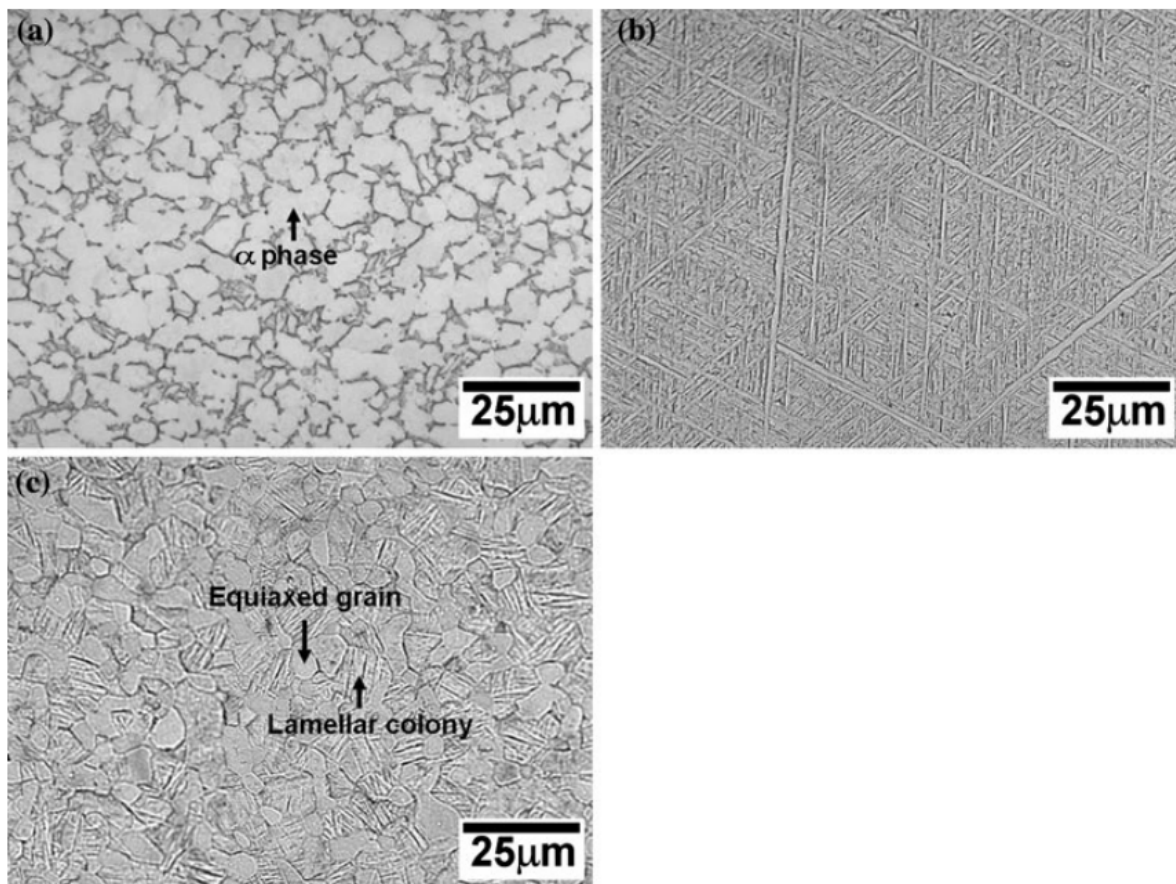

Figure 7 - Micrograph images of samples of Ti-6Al-4V with equiaxed (a), lamellar (b), and bimodal (c) phase arrangements. Reprinted from [11].

3   Impact of Microstructure on Mechanical Properties

The different microstructures of titanium and its alloys have a significant effect on the bulk properties of the material. These differences in microstructure impact a number of mechanical properties – including tensile, creep, and fracture properties – and controlling these properties is important for the development and production of successful alloys. This section will present a discussion of how the microstructural features described in Section 2 influence the mechanical properties of the bulk alloy.

3.1   Ductility

For pure titanium, the beta phase has more slip systems and a shorter minimum slip path than the alpha phase, as previously discussed in Section 2.1.1 [1]. More slip systems and a shorter slip path make it easier for dislocations to move throughout a material, and consequently beta phase titanium tends to be more ductile than alpha phase titanium.

The presence of alloying elements in titanium tends to decrease material ductility. This is due to the pinning phenomenon introduced in Section 2.2.1, which impedes the movement of dislocations in a material [1] [9]. However, for alpha+beta alloys, the microstructural arrangement of the phases has a marked effect on the material's ductility. In the alpha+beta phase, bimodal phase arrangements tend to have the best ductility [4]. Additionally, the effective slip length for a material scales with the size of the phase grains within the alpha+beta structure [1] [7] [10]. Therefore finer structures, which give a smaller effective slip length, have increased ductility since dislocations can move more easily.

3.2   Strength

While the pinning phenomenon introduced in Section 2.2.1 decreases ductility, it significantly increases the material strength [1] [7] [12]. Because the introduction of alloying elements increases the resistance for dislocation movement, alloyed materials are significantly stronger than their unalloyed counterparts [6] [7]. This leads to a common trade-off between strength and ductility in alloyed materials, where increase in concentration of alloying elements leads to an increase in material strength and a decrease in the material ductility.

3.3   Creep

A number of mechanisms control the creep of materials over time. One important mechanism is diffusion controlled, where dislocations diffuse through a lattice, causing material elongation [6]. Another is controlled by the presence of internal obstacles within a crystal, which can slow the movement of dislocations [6].

When comparing the alpha and beta phases of titanium, the significantly smaller diffusion coefficient and greater number of internal obstacles to dislocation movement (due to longer minimum slip path and fewer slip systems) make the alpha phase significantly more creep resistant [1]. For alpha+beta titanium, the arrangements of the phases can lead to a wide range of creep resistances [4]. The lamellar arrangement of alpha+beta titanium has the best creep resistance, due to the presence of alpha-phase lamellae and the obstacles that the boundaries between lamellae colonies present to dislocation movement [4] [10]. Additionally, thinner alpha lamellae colonies create more obstacles to dislocation movement than thicker lamellae, and result in improved creep resistance [4].

3.4   Fracture

Fracture mechanics are governed by the resistance to crack growth within a material [7]. Materials with many internal obstacles tend to have increased fracture toughness since propagating cracks can be deflected [1]. Alpha+beta phase titanium typically has higher values for fracture toughness due to its two-phase, non-uniform structure with more internal obstacles than single phase titanium [1].

Among the possible alpha+beta phase arrangements, the lamellar phase arrangement typically shows the best fracture toughness [1] [10] [13]. The presence of alpha-lamellae colonies with varying orientations significantly hinders crack growth within materials by causing cracks to branch and change directions, both of which dissipate energy and prevent fracture [1] [13]. Additionally, microstructures with thinner alpha-lamellae exhibit improved fracture toughness due to the increased frequency of obstacles to crack growth (i.e. the boundaries of the lamellae) [13].

4   Analysis of Ti-6Al-4V

Titanium alloy Ti-6Al-4V is the most widely used and researched alloy of titanium. It contains 6% aluminum (an alpha stabilizer) and 4% vanadium (a beta stabilizer) as its alloying elements, as well as

small amounts of other impurities that might exist. This section will use Ti-6Al-4V as an example to explicitly evaluate the effects of alloying on bulk material properties.

4.1   Comparison of Bulk Material Properties for Ti-6Al-4V and its Constituents

A number of the material properties of titanium alloys are affected by the material's microstructure. Table 1 presents a comparison of a number of different room temperature bulk material properties and indices for Ti-6Al-4V and its pure constituent elements.

The final column of each row provides the calculated ratio between the property value for Ti-6Al-4V and pure titanium. The final two rows of the table include indices for minimizing the mass of a structure, depending on the structural loading scenario: 1) σ_{ty}/ρ, the mass minimizing index for a tension-loaded, strength-limited structure, and 2) $\sigma_{ty}^{1/2}/\rho$, the mass minimizing index for a bending-loaded, strength-limited structure [12].

Table 1 - Comparison of selected minimum material properties for Ti-6Al-4V and its constituent elements at room temperature. Data from [14].

	Pure Titanium	Pure Aluminum	Pure Vanadium	Ti-6Al-4V Alloy	Property Ratio, (Ti-6Al-4V / Pure Ti) [-]
Density, ρ [g cm^{-3}]	4.51	2.67	6.05	4.43	0.98
Tensile Strength, σ_{ty} [MPa]	240	76	215	862	3.59
Fracture Toughness, K_{Ic} [MPa m$^{1/2}$]	55	30	70	84	1.53
Ductility [-]	0.25	0.37	0.01	0.05	0.20
σ_{ty}/ρ [MPa kg^{-1} m^3]	0.053	0.028	0.036	0.195	3.68
$\sigma_{ty}^{1/2}/\rho$ [MPa$^{1/2}$ kg^{-1} m^3]	0.003	0.003	0.001	0.007	1.92

4.2   Discussion of Bulk Material Properties

The difference between the tensile strength, fracture toughness, and ductility for Ti-6Al-4V and pure titanium are significant, as can be seen by the ratios presented in the final column of Table 1. The effects of the microstructure on the material properties of Ti-6Al-4V follow the expected trends, as discussed generally in Section 3.

One of the largest changes in Ti-6Al-4V material properties happens for the ductility, which is reduced to 20% of its unalloyed value. This is due to the 6% aluminum and 4% vanadium in solution with titanium.

The presence of the alloying elements impedes the movement of dislocations in the material, thereby reducing its ductility, as introduced in Section 3.1.

There is also a large change in the tensile yield strength value between the alloyed and unalloyed forms of titanium. Similar to the underlying cause of the ductility change, alloying elements in the crystal lattice impede the movement of dislocations in the material. However, instead of the decrease in value for ductility, there is a significant increase of 3.59 times in the strength of the material. The strength of the Ti-6Al-4V alloy is greater than any of its constituent components, and is due to the effects of alloying elements on the local lattice stress field.

The change in fracture toughness is not as large as the changes in ductility and strength, but is still significant. The presence of the alpha-phase lamellae in the alpha+beta Ti-6Al-4V alloy contribute to the 1.53 times greater fracture toughness for Ti-6Al-4V as compared to pure titanium.

4.3   Discussion of Mass-Minimizing Indices

When selecting materials for aerospace structures, minimizing the mass is often a primary concern. The use of material indices, which are dependent on the loading scenario and limiting constraint, help to simplify the material selection process. Table 1 contains calculated values for two such material indices - σ_{ty}/ρ for tension-loaded, strength-limited structures and $\sigma_{ty}^{1/2}/\rho$ for bending-loaded, strength-limited structures – as previously described in Section 4.1.

Both of these indices depend on the material density. For aerospace applications, alloying titanium with aluminum is a popular choice, since it reduces the density of the alloy. Ti-6Al-4V is alloyed with 6% aluminum, which is less dense than titanium, and 4% vanadium, which is more dense. The resulting alloy has a density 98% percent that of pure titanium. It is a seemingly small difference, however even the small reduction in density can lead to large mass savings for aerospace vehicles.

The increase in the σ_{ty}/ρ material index for Ti-6Al-4V is even larger than the increase for strength alone, since now the reduction in density is factored in. The increase in the $\sigma_{ty}^{1/2}/\rho$ index is less large, although still significant. These indices help to show how important alloying can be for mass reduction for aerospace vehicles. The increase in strength due to the pinning phenomenon and the reduction in density due to alloying element selection allow Ti-6Al-4V material to create several-fold lighter structures than any of its constituent components.

5   Conclusion

Titanium and its alloys are an important class of materials for a number of industries, especially the aerospace industry. The two phases of titanium – the hexagonal close packed alpha phase and the body centered cubic beta phase – display many differences in material properties due to the unique features of their structures. When titanium is alloyed with other elements, it can form a two-phase alpha+beta microstructure, which can modify material properties even further.

The most widely used titanium alloy, Ti-6Al-4V, takes advantage of a number of alloying phenomena, including dislocation pinning and formation of alpha-lamellae colonies, in order to create a material with strength and fracture performance that significantly exceeds any of its constituents. This improved material performance with relatively low density for Ti-6Al-4V makes it a mass-saving material choice for many aerospace applications. Moving forward, the development of new titanium alloys that take greater advantage of different alloying elements and phenomenology will lead to even better material performance.

6   Works Cited

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