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Developing a phenomenological equation to predict yield strength from composition and microstructure in β processed Ti-6Al-4V

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Keywords
Artificial neural networks, Genetic algorithms, Monte Carlo simulations, Titanium alloys, Phenomenological equation, Yield strength

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Developing a phenomenological equation to predict yield strength from composition and microstructure in β processed Ti-6Al-4V

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Abstract

A constituent-based phenomenological equation to predict yield strength values from quantified measurements of the microstructure and composition of β processed Ti-6Al-4V alloy was developed via the integration of artificial neural networks and genetic algorithms. It is shown that the solid solution strengthening contributes the most to the yield strength (~80% of the value), while the intrinsic yield strength of the two phases and microstructure have lower effects (~10% for both terms). Similarities and differences between the proposed equation and the previously established phenomenological equation for the yield strength prediction of the α+β processed Ti-6Al-4V alloys are discussed. While the two equations are very similar in terms of the intrinsic yield strength of the two constituent phases, the solid solution strengthening terms and the ‘Hall-Petch’-like effect from the alpha lath, there is a pronounced difference in the role of the basketweave factor in strengthening. Finally, Monte Carlo simulations were applied to the
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Keywords: Artificial neural networks, genetic algorithms, Monte Carlo Simulations, titanium alloys, phenomenological equation, yield strength

Introduction

The establishment of phenomenological equations which is able to predict the mechanical properties of various metallic materials given their composition and microstructure has long been sought. For instance, various phenomenological hardening rules have been established to explain the plastic behavior of crystals [1-4]. Unfortunately, there are some difficulties which hinder the development of phenomenological equations in multi-component, multi-phase engineering alloys. The first and the most important one is generating a large high-fidelity database which guarantees that all the most influential parameters involved in a phenomenon are taken into account. As an example, in the case of solid solution strengthening of titanium alloys, the contribution of aluminum, oxygen, iron, etc. in strengthening must be considered [5]. The next problem is related to the complex relationship which may exist between parameters and their synergistic effects on the output. In this case, it is almost impossible in the laboratory scale to change only one parameter (e.g., aluminum content) and keep all the other parameters (e.g., colony scale factor) fixed at a constant value to reveal the effect of each parameter on the output (e.g., yield strength in titanium alloys).
A novel method to overcome the second problem and thus derive phenomenological equations was developed via the integration of artificial neural networks (ANN), genetic algorithms (GA) and Monte Carlo (MC) simulations. This method was applied successfully to predict the yield strength of $\alpha+\beta$ processed Ti-6Al-4V (weight percent) alloy with the maximum error in the prediction of yield strength of 4% [6]. The developed phenomenological equation is a function of both compositional variables (i.e., the concentration of oxygen, aluminum, iron, and vanadium) as well as microstructural variables (i.e., lath thickness, mean equiaxed alpha size, the volume fraction of equiaxed alpha, and the total volume fraction of the alpha phase). This integrated effort builds upon previous discrete efforts involving both artificial neural networks and genetic algorithms. Notably, artificial neural networks have been used extensively in determining the mechanical properties and the kinetics of the phase transformation of titanium [7-13], nickel [14] and steel [15-20]. Genetic algorithm has also been used broadly in materials science [21-24] to optimize parameters involved in a phenomenon [25, 26] and also microstructural evolutions [27, 28]. In some cases, GA has been integrated with ANN to optimize the results of a developed neural network model [29-31]. For instance, the heat treatment process of 7175 aluminum alloy was optimized according to the desired final properties via the integration of ANN and GA [32].

In order to achieve the desired microstructures (and mechanical properties), $\alpha+\beta$ titanium alloys are subjected to various thermomechanical processes. The characteristics of the microstructures of these alloys can be categorized as originating from either $\beta$ or $\alpha+\beta$ processing depending upon the temperature at which the thermomechanical processing is applied. If the thermomechanical processing is conducted above the beta transus temperature, the temperature at which beta phase ($\text{bcc}$ crystal structure) transforms to alpha phase ($\text{hcp}$ crystal structure), the
evolved microstructure is called β processed. Slow cooling rates of the β processed alloys result in colony microstructure in which Widmanstatten lath-like precipitates of alpha phase are arranged parallel to each other. A scanning electron microscope (SEM) image of a furnace-cooled β processed alloy is shown in Fig. 1. In this figure, the darker features are α laths and the brighter features are β ribs. High cooling rates results in the formation of a basketweave microstructure.

While the softest microstructure in the α+β processed alloy is equiaxed alpha particles and the hardest one is basketweave microstructure, the softer microstructure in the β processed alloys is the colony microstructure and the harder one is the basketweave microstructure. Colony size, alpha lath thickness and the interface of the α laths and β ribs are considered to be the microstructural parameters that most significantly affect the mechanical properties of β processed titanium alloys [33]. Notably, the contribution of prior beta grain size on the yield strength is deceptive. Kar et al. believe that the role of beta grain size should not be considered individually. It is deemed that in the larger beta grain sizes basketweave microstructure forms in the middle of the grains while in the smaller beta grain sizes only colony microstructure forms. As a result, yield strength reduces via beta grain size refinement [34]. From the crystallographic point of view, the Burgers orientation relationship (i.e., (0001).||(110), and [2Î10].||(111).) is satisfied between α laths and β ribs. This orientation relationship results in the easy activation of dislocation glide (slip transmission [35]) through the interface of α laths and β ribs [35], so long as the neighboring α lath shares a common crystallographic orientation (i.e., is in the same colony). As a result, yield strength is expected to be inversely proportional to the size (percentage) of colonies. Also, it has been previously reported that yield strength is inversely
proportional to the lath thickness in both $\alpha+\beta$ [13] and $\beta$ [34] processed titanium alloys. This is due to the fact that in the larger $\alpha$ laths, dislocations can move a longer distance without encountering any interfacial barrier.

In this work, initially an artificial neural network model was developed to capture the effect of the most influential variables (both compositional and microstructural variables) on the yield strength of $\beta$ processed Ti-6Al-4V alloy. A proposed phenomenological equation (very similar in many terms to the $\alpha+\beta$ processed phenomenological equation of [6]) was optimized using genetic algorithms, and then used to predict the yield strength of $\beta$ processed Ti-6Al-4V alloy. Importantly, the differences between the separately optimized $\beta$ and $\alpha+\beta$ processed equations are discussed. Lastly, Monte Carlo simulations were used to study the effect of uncertainties in the input measurements (e.g., aluminum content, etc.) on the yield strength of the equation developed for the $\beta$ processed $\alpha+\beta$ titanium alloys.

2. Methods

2.1 Experimental techniques

Nine compositionally different titanium alloys were made in the range of Ti-6Al-4V alloy (all compositions in weight percent). These alloys capture the extremes of the specification range. The systematic variation in the important elements, which were measured by Timet using inductively coupled plasma (ICP), are as follow:

\[
\text{Al: 4.76-6.55; V: 3.3-4.45; O: 0.07-0.20; Fe: 0.11-0.41}
\]
To exclude the effect of texture variation on the yield strength in this study, all the samples included in the database were cut from the same radius of round billets. It should be noted although texture can affect the yield strength remarkably, it is not considered as an input variable in the phenomenological equation developed in this study due to the limited number of available samples. However, it is worth noting that there are statistical methods to reveal the effect of texture on the mechanical properties. While not a part of this effort, such methods can be applied to the phenomenological equation developed in this study to improve the accuracy of yield strength predictions via considering the effect of texture on the mechanical properties.

All the samples were elongated uniaxially, sectioned, and prepared for microscopy analyses by conventional metallographic methods. Samples were characterized by an optical microscope as well as a FEI FEG Sirion scanning electron microscope (SEM) operating in backscattered electron imaging mode at 15 kV with a 3 nm spatial resolution. The input variables in the phenomenological equation are the volume fraction of total alpha, percent of colony, α-lath thickness and the concentrations of aluminum, vanadium, iron and oxygen. The microstructural features were quantified using stereological methods described elsewhere [36]. The output of the phenomenological equation is yield strength.

2.2 Computational approach

Artificial neural networks, genetic algorithms and Monte Carlo simulations were integrated to derive a phenomenological equation to predict the yield strength of α+β titanium alloys from a dataset containing the aforementioned variables (Fig. 2). The integration method and the way that the phenomenological equation is derived are explained in detail in another publication [6].
In brief, the database was divided into two parts containing two thirds of the database (called the training dataset) to create the ANN model and one third of the database (called the testing dataset) to evaluate the ANN model. A committee model was developed, using Bayesian neural network code developed by David Mackay [37, 38], from the best three models among 1500 proposed ANN models. Also, virtual experiments were conducted in which all the variables were constant at their average values and only one variable was changing from its minimum value to its maximum value. Such virtual experiments were conducted in order to reveal the individual effect of each variable on the output (e.g., yield strength) via applying the developed ANN committee model to the virtual datasets. Unfortunately, the ANN model is not a phenomenological model; i.e., it is only a summation of some hyperbolic tangent functions and it cannot be interpreted based on physical metallurgy principles.

Genetic algorithms, as an optimization tool to find the global extrema, was used in this study to derive a phenomenological equation from the original dataset. Initially, a phenomenological equation that incorporates known physical dependencies is proposed to predict the yield strength. For example, in a single-phase material where the microstructural features do not impact the attending mechanical properties, one might assumed that the total yield strength is the summation of the intrinsic yield strength and any solid solution strengthening that may be present. In the Ti-6Al-4V discussed here, such terms would include the intrinsic yield strength values of the alpha and beta phases as well as solid solution strengthening (SSS) due to the presence of Al and O in the alpha phase and V and Fe in the beta phase (Eq. 1),

\[
\sigma_{ys} (MPa) = (\sigma_{0}^{\alpha} F_{\alpha}^{\alpha} + (\sigma_{0}^{\beta} F_{\beta}^{\beta}) + F_{V}^{\alpha} (A_{\alpha} C_{Al}^{n_{\alpha}} + A_{O} C_{O}^{n_{\alpha}}) + F_{V}^{\beta} ((A_{V} C_{V}^{n_{V}})^{n_{1}} + (A_{Fe} C_{Fe}^{n_{Fe}})^{n_{2}})^{n_{3}} + SSS^{\alpha} + SSS^{\beta} \]

(1)
where \( \sigma_0^X \), \( F_V^X \) and \( C_Y \) are the intrinsic yield strength of phase X, volume fraction of phase X and the concentration of Y element, respectively. Finding the optimum precursors and powers of Eq. 1 (i.e., \( A \) and \( n \)) leads to predicting the yield strength based upon the dataset inputs (e.g., Al content, etc.) within an acceptable level of accuracy. This precursor/power optimization can be conducted using GA. The proposed equation can be modified in a trial and error process; i.e., dropping some terms if their contributions to the yield strength are negligible or adding some new terms to make the predictions more accurate. In this paper, this process is called the equation-construction process, and includes descriptors of the microstructural features in addition to the terms given above. Also, the optimized equation can be evaluated through comparing the results of ANN virtual experiments with the yield strength values estimated by the optimized equation for the virtual datasets.

Finally, Monte Carlo simulations were applied to study the effect of uncertainties in the input measurements on the output (i.e., yield strength). The average of the standard deviation of each measurement (e.g., lath thickness) was assigned as the uncertainty value of the measurement for that variable. In this study, the maximum deviation of the yield strength from the value estimated by GA was determined through a 3000-iteration Monte Carlo simulation for each variable.

3. Results and discussion

3.1. The proposed equation

Initially, the ANN model was developed using the original dataset. The established committee model was able to estimate the yield strength of the raw data with the maximum error of 3% with respect to the measured yield strength values (Fig. 3). The ANN committee model provided the opportunity to independently study the effect of each variable (e.g., Al content) on the yield
strength via conducting virtual experiments. To derive the phenomenological equation through the integration of ANN and GA, it was assumed ‘primarily’ that the previously proposed equation for the yield strength prediction of $\alpha+\beta$ processed Ti-6Al-4V alloy [6] is valid with a minor correction which is the elimination of the extraneous equiaxed alpha term from the equation. The proposed equation for estimating the yield strength of $\alpha+\beta$ processed Ti-6Al-4V alloy is presented in Eq. 2,

$$
\sigma_{ys} (MPa) = (\sigma_{0}^\alpha * F_{V}^\alpha) + (\sigma_{0}^\beta * F_{V}^\beta) + \text{Two-phase composite of intrinsic strength}
$$

$$
F_{V}^\alpha (A_{Al} * C_{Al}^{n\alpha} + A_{O} * C_{O}^{n\beta}) + \text{Solid solution strengthening (hcp alpha)}
$$

$$
F_{V}^\beta ((A_{V} * C_{V}^{n\beta})^{n_{V}} + (A_{Fe} * C_{Fe}^{nFe})^{n_{V}}) + \text{Potential synergistic solid solution strengthening (bcc beta)}
$$

$$
k_{y,\text{equiaxed}}^{\alpha} * F_{V}^{\text{equiaxed},\alpha} * \text{Equiaxed size}^{-n_{y}} + \text{Hall-Petch effect (equiaxed alpha particles)}
$$

$$
(1 - F_{V,\text{equiaxed}}^{\alpha}) \frac{\text{Colony}}{100} * k_{y,\text{lath}}^{\alpha} * LW^{-n_{y}} * (RT)^{n_{3}} + \text{Hall-Petch effect (alpha lath)}
$$

$$
(1 - F_{V,\text{equiaxed}}^{\alpha}) \frac{100 - \text{Colony}}{100} * B * \text{SSS} \text{Basketweave factor}
$$

where $\sigma_{0}^{X}$ is the intrinsic yield strength value of phase X, $F_{V}^{X}$ is the volume fraction of X, $A_{X}$ is the precursor used in the solid solution strengthening term of element X, $C_{X}$ is the concentration of element X, $n_{X}$ is a power, $k_{y}^{X}$ is the Hall-Petch constant associated with X, LW is the width of an alpha lath, B is a constant used in the basketweave factor term and SSS is the solid solution strengthening of the alpha and beta phases. Notably, $RT$ represents rib thickness which can be determined based on stereological methods following Eq. 3 [6],

$$
RT = Lathwidth * (1 - (F_{V}^{\alpha} - F_{V,\text{equiaxed}}^{\alpha})) \text{ Eq. 3}
$$
where $F^\alpha_V$ is the total volume fraction of the alpha phase which forms colony, basketweave and equiaxed alpha microstructures.

The capability of the modified equation to predict the yield strength of the $\beta$ processed Ti-6Al-4V alloy was evaluated in two ways, namely (1) comparing the measured yield strength values with the GA predicted values for the raw database and (2) comparing the virtual experiment results of the ANN model with the GA predicted values. To cover all the aspects of the strengthening mechanisms in the $\beta$ processed alloy and increase the accuracy of the yield strength estimations by the phenomenological equation, some new terms were added during the equation-construction process. Based on the results of the current study, Eq. 4 was proposed which represents all the most influential terms involved in the strengthening of the $\beta$ processed Ti-6Al-4V alloy,

$$
\sigma_{ys} (MPa) = (\sigma_0^\alpha * F^\alpha_V) + (\sigma_0^\beta * F^\beta_V) + 
\sigma_0^\alpha + \sigma_0^\beta 
$$

$$
F^\alpha_V * (A_{Al} * C_{Al}^{n_{Al}} + A_O * C_{O}^{n_0}) + 
SSS^\alpha 
$$

$$
F^\beta_V * ((A_{Fe} * C_{Fe}^{n_{Fe}})^{n_0} + (A_{Fe} * C_{Fe}^{n_{Fe}})^{n_2})^{n_3} + 
SSS^\beta 
$$

$$
PC * B * LW^{-n_4} * (LW * \frac{1 - F^\alpha_V}{F^\alpha_V})^{n_4} + 
\text{Hall-Petch effect (alpha lath)}
$$

$$
C * LW * (\frac{1 - F^\alpha_V}{F^\alpha_V})^{n_5} + 
\text{Constrained beta}
$$

$$
\frac{100 - \text{Colony} * D * SSS}{100} + 
\text{Basketweave factor}
$$

$$
E * \frac{\text{Colony} * CSF^{n_6}}{100} 
\text{Colony scale factor}
$$

where $B$, $C$, $D$ and $E$ are constants. The remaining parameters are the same as those introduced in Eq. 2.
There are 20 unknown variables in Eq. 4, specifically $\sigma_0^\alpha, \sigma_0^\beta, A_{Al}, n_{Al}, A_{O}, n_{O}, A_{V}, n_{V}, A_{Fe}, n_{Fe}, n_2, n_3, B, n_4, C, n_5, D, E$ and $n_6$. Considering the two mentioned evaluation methods, GA determined all these unknown variables in a way that the developed phenomenological equation estimates the yield strength values of the raw data with the maximum error of 5% with respect to the measured values (Fig. 4). The developed phenomenological equations for the $\alpha+\beta$ [6] and $\beta$ processed Ti-6Al-4V alloys are presented in Table 1. As stated previously, the phenomenological equation derived for the $\beta$ processed Ti-6Al-4V alloy was evaluated via comparing the ANN and GA virtual experiment results. There is a nice consistency between the virtual experiment results of the hyperbolic tangent functions (ANN approach) and the phenomenological equation (GA approach) for all the variables except vanadium (Fig. 5 and Fig. 6). The discrepancy exists for the case of vanadium is due to the fact that in the developed phenomenological equation the contribution of vanadium to the total yield strength is considered only in the solid solution strengthening. However, vanadium plays a significant role in the formation of basketweave microstructure [39]. Unfortunately, the latter contribution cannot be captured via the currently proposed phenomenological equation as the nature of the contribution is different.

In the last step of integrated approach, MC method was applied to the phenomenological equation to study the effect of measurement uncertainties on the yield strength values. The MC results associated with the compositional and microstructural variables are depicted in Fig. 7 and Fig. 8, respectively. Interestingly, the MC method shows that it is possible to interpret the difference between GA and ANN predicted yield strengths as effectively zero, and consequently indicates that GA and ANN delineate the same multi-variable model with two different representations (e.g., phenomenological and hyperbolic tangent), only by slightly changing the measured values within the range of their measurement error as presented by ‘Applying MC to
GA-ANN’ lines in Fig. 7 and Fig. 8. As an example, the variation of the Al content within the measurement error (i.e., new Al content = measured Al content ± measurement error) results in a range of yield strength values estimated by the developed phenomenological equation. ‘Applying MC to GA-ANN’ line indicates the minimum difference between the yield strength value predicted by the ANN model and all of these estimated yield strength values, Fig. 7(a). Also, to indicate the range of yield strength variation via considering the measurement errors, the maximum difference between the values predicted by the phenomenological equation with and without applying the MC method was added to the values estimated by the phenomenological equation for the raw database without considering the measurement uncertainties. These new values were called ‘GAplus’. Similarly, ‘GAmminus’ was made via subtracting the maximum difference value from the yield strength values predicted by the phenomenological equation. To show the maximum range of yield strength discrepancies between ANN and the phenomenological equation, ‘GAplus’ and ‘GAmminus’ were subtracted from the ANN predicted values as shown in Fig. 7 and Fig. 8. Analogous to ‘GAplus’, the error bar values determined by the Bayesian neural network code (presented in Fig. 5 and Fig. 6) were added to the ANN predicted yield strength values. The new values were called ‘ANNplus’. Similarly, the error bar values were subtracted from the ANN predicted values and they were called ‘ANNminus’. The difference between the values predicted by the phenomenological equations and ‘ANNplus’ as well as ‘ANNminus’ are presented in Fig. 7 and Fig. 8.

The sensitivity analyses of the contribution of the microstructural and compositional variables on the total yield strength of the β processed Ti-6Al-4V are given in Table 2. Similar to the phenomenological equation developed for the α+β processed alloys, the compositional variables have a major contribution in the total yield strength.
3.2. Similarities between β and α+β processed phenomenological equations

Interestingly, the intrinsic yield strength values of alpha phase (89 MPa) and beta phase (45 MPa) in both equations are exactly the same which result in alike contribution in the total yield strength (Fig. 9). This is an important observation, as it shows that the optimization routines conducted on both databases indicates the same intrinsic strength of the material. It also suggests that there is little difference in either texture or Taylor (work) hardening. These terms, though not included in these efforts, would be ‘remainders’ attached to the intrinsic yield strength terms. The precursors and powers of the solid solution strengthening of Al, O, V and Fe are very similar in the both equations. The dissimilarities in the solid solution strengthening terms of these two equations result in ~13 MPa (i.e., less than 2% of the total yield strength) difference in the calculated contribution of Al in solid solution strengthening. Analogously, the difference between the contributions of O, V and Fe in the solid solution strengthening term of the two equations is less than 0.7%, 0.2% and 0.5% of the total yield strength, respectively. The small difference in the contribution of the solid solution strengthening in the total yield strength is shown in Fig. 9, along with the contribution of the other terms. For the case of microstructure effect on the yield strength, since basketweave microstructure is the hardest microstructure in both α+β and β processed titanium alloys, it is expected to have similar terms in α+β and β processed equations, though yielding is dominated by the weakest features. In reality, equiaxed alpha microstructure does not form in the β processed titanium alloys, therefore the basketweave factor term of the β processed equation is only a simplified version of the α+β processed equation. As shown in Fig. 9, the contributions of the Hall-Petch alpha lath term in the strengthening of α+β and β processed Ti-6Al-4V alloys is almost equivalent. An extensive discussion on the contribution of the intrinsic yield strength, the solid solution strengthening and
basketweave factor on the total yield strength of the $\alpha+\beta$ processed titanium alloys is given elsewhere [6]. Some of the most salient points are mentioned briefly.

- In a multi-phase material, a rule of mixtures incorporating phase fractions ($F_v$) may be adopted

- The yield strength of a well-annealed elementally pure titanium has been reported as 78.45 MPa [40]. This value does not include any potential texture terms. The values for the individual slip systems range from 49 MPa to 110 MPa [41]. The value reported in [40] and that determined in the previous study and here (i.e., 89 MPa) are consistent with this previous data.

- Since beta phase titanium is not stable at room temperature, no experimental value is available in the literature. However, since the number of slip systems in bcc crystal structure is more than hcp crystal structure, a lower value of the yield strength for the beta phase in comparison to the alpha phase is expected.

- Experimental observations about the strengthening effect of solute atoms in titanium revealed that the order of strengthening contribution is $O>Fe>Al>V$ [5], the same as determined previously and shown here.

- The postulated forms for solid solution strengthening are different for the alpha and beta phases. Alpha phase has only one substitutional atom (Al) and one interstitial atom (O), resulting in a simple additive term. However, beta phase has two substitutional atoms (V and Fe), requiring that possible synergistic effects to be considered. The model developed in [6] demonstrated that it was unlikely V and Fe behaved in a synergistic manner.

- The values calculated for the strengthening contributions of Al and O elements are consistent with the experimental data obtained by Williams et al. [42].
3.3. Differences between $\beta$ and $\alpha+\beta$ processed phenomenological equations

As stated previously, the expected microstructures of the $\alpha+\beta$ processed alloys are equiaxed alpha, colony and basketweave microstructures. In this case, equiaxed alpha and basketweave microstructures are the softest and hardest ones, respectively. However, in the $\beta$ processed samples equiaxed alpha microstructure does not exist. Thus, the Hall-Petch strengthening of equiaxed alpha grains is a vestige and thus is eliminated in the $\beta$ processed equation. Another difference between the two equations arises from the effect of beta rib thickness on the yield strength. As the beta ribs become increasingly constrained by the neighboring alpha laths as their thickness decreases, the strength does increase. Initially, the constrained beta strengthening term was a part of the $\alpha+\beta$ processed equation. GA assigned a negligible contribution to this term – as the deformation is dominated by the equiaxed $\alpha$ particles. However, GA revealed that this term has around 2.4% contribution in the total yield strength of $\beta$ processed Ti-6Al-4V alloy as depicted in Fig. 9. The final difference between the microstructures is the presence of the basketweave microstructure. The basketweave microstructure can be described as the interweaving of multiple alpha lath variants whereas the colony microstructure can be described as parallel and adjacent alpha laths of the same variant. This difference results in a difference in strength, owing to hindered slip transmission arguments. The basketweave microstructure is generally observed to be stronger than the colony microstructure. Given the absence of equiaxed alpha particles and the increased volume fraction of basketweave in the complete dataset, it is not surprising that the basketweave term plays a more important role in the $\beta$ processed equation.
4. Conclusions

1. The integration of ANN and GA provides a method which is used to derive phenomenological equations from a high fidelity database.

2. The derived equation for the prediction of yield strength in β processed titanium alloys is in close agreement with the similar equation developed for α+β processed titanium alloys, although it is microstructurally distinct.

3. As expected, the similarities of the two equations are intrinsic yield strength values, solid solution strengthening terms and the Hall-Petch effect of alpha lath.

4. The main difference between the two equations arises from the fact that equiaxed alpha microstructure (which is a softest microstructure) does not exist in the β processed titanium alloys and the softer microstructure is colony.

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Figure 1. SEM micrographs of a β processed colony microstructure is shown.
Figure 2. Schematic of the integration approach is shown (adopted from [6]).
Figure 3. Yield strength values estimated by the developed ANN committee model are in close agreement with the measured yield strength values for the training and testing datasets.

Figure 4. The GA-developed phenomenological equation estimated the yield strength of the raw database with the maximum error of 5%.
Figure 5. Compositional virtual dependencies of (a) aluminum (b) vanadium (c) iron and (d) oxygen are depicted.
Figure 6. Microstructural virtual dependencies of (a) volume fraction of total alpha (b) percent colony and (c) lath thickness are shown.
Figure 7. Monte Carlo results for (a) aluminum (b) vanadium (c) iron and (d) oxygen are presented.
Figure 8. Monte Carlo results for (a) volume fraction of total alpha (b) percent colony and (c) lath thickness are presented.
Figure 9. Contribution comparison of the most influential terms involved in the strengthening of \(\alpha+\beta\) and \(\beta\) processed Ti-6Al-4V alloys is shown.

Table 1. Comparison of the \(\beta\) processed equation with the \(\alpha+\beta\) processed equation

<table>
<thead>
<tr>
<th>Parameters</th>
<th>(\beta) processed equation</th>
<th>(\alpha+\beta) processed equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\sigma^\alpha_0 + \sigma^\beta_0)</td>
<td>((89 * F_V^\alpha) + (45 * F_V^\beta))</td>
<td>((89 * F_V^\alpha) + (45 * F_V^\beta))</td>
</tr>
<tr>
<td>(SSS^\alpha)</td>
<td>(F_V^\alpha * (145C_{Al}^{0.667} + 764C_O^{0.667}))</td>
<td>(F_V^\alpha * (149.5 * C_{Al}^{0.667} + 745 * C_O^{0.667}))</td>
</tr>
<tr>
<td>(SSS^\beta)</td>
<td>(F_V^\beta * ((45C_V^{0.7})^{0.5} + (237C_{Fe}^{0.7})^{0.5})^2)</td>
<td>(F_V^\beta * ((34 * C_V^{0.765})^{0.5} + (245 * C_{Fe}^{0.765})^{0.5})^{2.15})</td>
</tr>
<tr>
<td>Hall – Petch effect of equiaxed alpha particles</td>
<td>(Not applicable)</td>
<td>(110 * F_V^{\text{equiaxed}_-\alpha} * \text{Equiaxedsize}^{-0.5})</td>
</tr>
</tbody>
</table>
Table 2: Sensitivity assessment of compositional and microstructural variables on the yield strength of β processed Ti-6Al-4V alloy (all stress units in MPa)

<table>
<thead>
<tr>
<th></th>
<th>$\sigma_0$</th>
<th>$\sigma_{ss}$</th>
<th>$\sigma_{HP}$ (α lath)</th>
<th>Constrained beta</th>
<th>Basketweave factor</th>
<th>Colony scale factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Avg. % of $\sigma_{ss}$</td>
<td>10.5</td>
<td>78</td>
<td>5.4</td>
<td>2.4</td>
<td>3.4</td>
<td>0.3</td>
</tr>
<tr>
<td>Avg. effect</td>
<td>83.9</td>
<td>628</td>
<td>43.3</td>
<td>19.4</td>
<td>29</td>
<td>2.3</td>
</tr>
<tr>
<td>Min. effect</td>
<td>81.4</td>
<td>524</td>
<td>11.2</td>
<td>6.8</td>
<td>0</td>
<td>0.5</td>
</tr>
<tr>
<td>Max. effect</td>
<td>86</td>
<td>739.4</td>
<td>64.4</td>
<td>30.7</td>
<td>136.6</td>
<td>3.6</td>
</tr>
</tbody>
</table>
References