Physics-Based Machine-Learning Approach for Modeling the Temperature-Dependent Yield Strength of Superalloys

Baldur Steingrimsson,∗ Xuesong Fan, Benjamin Adam, and Peter K. Liaw

In the pursuit of developing high-temperature alloys with improved properties for meeting the performance requirements of next-generation energy and aerospace demands, integrated computational materials engineering has played a crucial role. Herein, a machine learning approach is presented, capable of predicting the temperature-dependent yield strengths of superalloys utilizing a bilinear log model. Importantly, the model introduces the parameter break temperature, \( T_{\text{break}} \), which serves as an upper boundary for operating conditions, ensuring acceptable mechanical performance. In contrast to conventional black-box approaches, our model is based on the underlying fundamental physics built directly into the model. A technique of global optimization, one allowing the concurrent optimization of model parameters over the low- and high-temperature regimes, is presented. The results presented extend previous work on high-entropy alloys (HEAs) and offer further support for the bilinear log model and its applicability for modeling the temperature-dependent strength behavior of superalloys as well as HEAs.

1. Introduction

The conventional approach to alloy design assumes selecting a main component based on the primary property needed in the alloy, with one or more additions to provide secondary properties. For over six decades, superalloys have provided reliable and cost-effective means for achieving high operating temperatures and stress conditions, first in aircraft and later in industrial gas turbines.\(^1\) The zenith of superalloy development was in the 1960s, as columnar grain alloys and single crystals were then made feasible, and many polycrystalline alloys matured into commercial reality.\(^1\) Since then, advances in powder metallurgy processing, single-crystal and directionally solidified alloy designs, and oxide-dispersion strengthening have ensued, along with advances in additive manufacturing and integrated computational materials engineering.

In the case of nickel-based superalloys, nickel is selected as the main component because of its high melting point. Nevertheless, chromium is added to prevent corrosion, and titanium and aluminum are included to increase strength. The Ni-based superalloys can accommodate \( \gamma, \gamma', \gamma'' \), carbides, or topologically closed-packaged (TCP) phases, as explained in the Supporting Information. Co-based superalloys can similarly contain \( \gamma, \gamma' \), carbide, or TCP phases. The Co-based superalloys are usually strengthened by a combination of carbides and solid-solution hardening.\(^1\) The use of steels for applications necessitating superalloys may also be of interest, as further explained in the Supporting Information, because certain steels have exhibited creep and oxidation resistance close to that of the Ni-based superalloys, while being much less expensive to manufacture.

Machine learning (ML) and data analytics, coupled with physics-based modeling, can assist with the effective search of the compositional space of superalloys and with the optimization of thermomechanical postprocesses. Figure 1 outlines the multiple sources that affect the mechanical properties of superalloys. As opposed to specifically applying ML, narrowly defined in terms of multivariate regression, single-layer or multi-layer neural networks, Bayesian graphical models, random forest models, support vector machines (SVMs), or decision trees, to the identification of superalloy compositions of interest, we reformulate the task in the broader context of engineering optimization.\(^2\)–\(^4\)

We recommend selecting an optimization technique suitable for the application at hand and the data available, but we certainly include ML in the consideration. Our rationale is based in part on observations from Agrawal et al.\(^5\) According to Table 2 and Figure 5 of ref. [5], there is at most a difference of a few percentages between the techniques applied to model the fatigue strengths of stainless steels. Specifically, in terms of the coefficient of correlation, \( R^2 \), which represents the variance explained by the model, a decision table method produced the \( R^2 \) of 0.901, an instance-based \( K \)-nearest neighbor (IBK) method an \( R^2 \) of 0.902. An ML approach also could clearly deliver higher \( R^2 \) values, but on the other hand, we also need to ensure that we can predict the mechanical properties of the target material. In the case of superalloys, the conventional approach to alloy design assumes selecting a main component based on the primary property needed in the alloy, with one or more additions to provide secondary properties.T
0.920, an instance-based $K$-nearest neighbor method with entropy-based distance function (Kstar) an $R^2$ of 0.941, a linear regression method with nonlinear transformation of certain input variables (LRTrans) method an $R^2$ of 0.959, a robust fit regression (RobustFitLSR) method an $R^2$ of 0.961, a linear regression method an $R^2$ of 0.963, a pace regression method an $R^2$ of 0.963, an artificial neural network method an $R^2$ of 0.972, a reduced error pruning tree (REPTree) method an $R^2$ of 0.972, a M5 model tree method (a conventional decision tree method with the option of linear regression functions at the nodes) an $R^2$ of 0.978 and a multivariate polynomial regression method an $R^2$ of 0.980, according to Table 2. Here, fatigue dataset for steel from the National Institute of Material Science was analyzed. The fatigue dataset consisted of 437 instances/rows, 25 features/columns (composition and processing parameters), together with a single target property (fatigue strength). The 437 instances comprised of 371 instances of carbon and low-alloy steels, 48 instances of carburizing steels, and 18 instances of spring steels. For further background information on the application of ML to the modeling of mechanical properties of alloys and on the motivation for coupling with physics-based modeling approaches, refer to refs. [2–4].

This paper introduces a bilinear log model for predicting the yield strength (YS) of superalloys across temperatures. It consists of separate exponentials for a low-temperature and a high-temperature regime, with a break temperature, $T_{break}$, in between. The underlying physics is accounted for, e.g., through diffusion processes required to initiate phase transformation processes in the high-temperature regime. Moreover, we show how piecewise linear regression can be employed to extend the model beyond two exponentials and yield accurate fit, in the case of a nonconvex objective function caused by hump(s) in the data. [3] Previous models for the temperature dependence of YS only accounted for a single exponential. [7, 36] However, the break temperature is crucial for the optimization of the high-temperature properties of alloys. For reliable operation, the temperature of turbine blades or disks (rotors) made from refractory superalloys may need to stay below $T_{break}$. Once the temperature increases beyond $T_{break}$, the superalloys can lose strengths rapidly due to rapid diffusion, facilitating dislocation motion and dissolution of strengthening phases. [36] We consider $T_{break}$ a crucial parameter in the design of superalloys with tailored high-temperature properties, one warranting the inclusion in the superalloy specifications. Hence, it is of paramount importance to be able to estimate $T_{break}$ accurately, e.g., using the global-optimization approach presented in prior works by Steingrimsson et al. [3]

In terms of impacts, this paper addresses a physics-based, i.e., not a black box, approach to ML and data analytics. Preference to such approaches, especially for applications involving materials science, may primarily stem from the fact that they involve fewer parameters than the black-box models and hence require less input data. With experiments often being time-consuming and expensive, in the case of such applications, high-quality input data tend to be a scarce resource. Moreover, the physics-based modeling approaches help establish causal links between output observations and the behavior of the underlying material system.

2. Results and Discussion

Figure 1 summarizes the multiple sources that impact the mechanical properties of superalloys. It bears noting that improvements in the YS may come at the expense of other properties. Hence, we have suggested a framework for joint optimization. [2–4] For instance, there typically is a trade-off between the ductility and the strength of the superalloys. Figure 1 presents an inverse design process, where components of the design are explicitly calculated from the target performance metrics provided.

For 40 superalloy compositions, Table 1 compares the performance of the bilinear log model to that of a model based on a single exponential. When averaged over these 40 compositions, the bilinear log model results in a mean squared error (MSE) of 0.00175 in the logarithmic domain, compared to the MSE of 0.0525 for the model based on a single exponential. This difference is exacerbated in the linear domain, where the bilinear log model yields the MSE of only 4,151 MPa², compared to the MSE of 25 836 MPa² for the model based on a single exponential. Analogous to Wu et al., [7] we employ a model with a single exponential for the overall YS, $\sigma_y(T)$, of the form

$$\sigma_y(T) = \sigma_a \exp \left( -\frac{T}{C} \right) + \sigma_b$$

where $\sigma_a$, $C$, and $\sigma_b$ represent fitting coefficients.

In an effort to identify superalloy compositions exhibiting the ability to retain strengths at high temperatures, we present Figure 2 and 3. The strengths of most metals tend to decrease with temperature, as dislocation motion becomes thermally activated. [39] In the case of high-temperature applications, one may look to derive a model of the form

$$YS = h(\text{composition}, T)$$

for the prediction of the YS of the superalloys across temperatures.

The strength vs temperature data presented in Figure 2–4 does not suggest a linear relationship but rather an exponential one. Therefore, a multivariate linear regression may not constitute a preferred approach. Figure 2–4 exhibit a high-temperature and a
Table 1. Quantification of the ability of superalloy compositions to retain yield strengths at high temperatures. $T_{\text{break}}$ refers to the breaking point between bilinear log models, defined in Equation (10).

| No. | Alloy | Category | Solvus temperature [$^\circ$C] | $T_{\text{break}}$ [$^\circ$C] | MSE: two exponentials | MSE: tingle exponential |
|-----|-------|----------|-------------------------------|-----------------------------|---------------------|-----------------------|
|     |       |          |                               |                             | Log    | Linear   | Log    | Linear |
| 1   | Waspaloy | Ni-base (precipit. hard.) | 1330                          | 755.2                       | 6.367e-04 | 5118     | 0.0070 | 44 260 |
| 2   | Udiment D979 | Fe-Ni-base (precipit. hard.) | 1390                          | 717.7                       | 0.005391 | 7678     | 0.0138 | 36 204 |
| 3   | Udiment 720 | Ni-base (precipit. hard.) | 1371                          | Not enough high-temp data pts. |                       |                      | 0.00056 | 243 720 |
| 4   | Udiment 520 | Ni-base (precipit. hard.) | 1371                          | 728.6                       | 5.663e-05 | 2221     | 0.0162 | 50 701 |
| 5   | Udiment 500 | Ni-base (precipit. hard.) | 1360                          | 748.9                       | 7.901e-05 | 1331     | 0.0181 | 48 108 |
| 6   | Astroloy | Ni-base (precipit. hard.) | 1399                          | 760.6                       | 5.759e-04 | 6643     | 0.0091 | 80 097 |
| 7   | Incoloy 825 | Fe-Ni-base (solid sol.) | 1370                          | 727.6                       | 3.196e-07 | 14       | 0.0367 | 2,198  |
| 8   | Inconel 807 | Fe-Ni-base (solid sol.) | 1275                          | 774.1                       | 1.069e-04 | 1358     | 0.00136 | 3,442  |
| 9   | Inconel 802 | Fe-Ni-base (solid sol.) | 1372                          | 760.0                       | 0.00252    | 1049     | 0.00495 | 2,248  |
| 10  | Inconel 801 | Fe-Ni-base (solid sol.) | 1372                          | Not enough high-temp data pts. |                       |                      | 0.00009 | 10 504 |
| 11  | Inconel 800 | Fe-Ni-base (solid sol.) | 1357                          | 675.8                       | 4.131e-04 | 637      | 0.00163 | 2,364  |
| 12  | Inconel 800 | Fe-Ni-base (solid sol.) | 1357                          | Not enough high-temp data pts. |                       |                      | 0.00623 | 699.8  |
| 13  | Inconel X750 | Ni-base (precipit. hard.) | 1393                          | Not enough high-temp data pts. |                       |                      | 0.00000 | 90 438 |
| 14  | Inconel 718 | Ni-base (precipit. hard.) | 1260                          | 717.3                       | 0.01707    | 7622     | 0.00819 | 58 230 |
| 15  | Inconel 625 | Ni-base (solid sol.) | 1290                          | 766.8                       | 2.911e-04 | 598      | 0.01615 | 14 501 |
| 16  | Inconel 917 (sheet) | Ni-base (solid sol.) | 1332                          | 893.4                       | 0.00201    | 2790     | 0.00235 | 4,010  |
| 17  | Inconel 601 | Ni-base (solid sol.) | 1360                          | 735.0                       | 7.862e-04 | 99       | 0.18572 | 7,360  |
| 18  | Inconel 600 | Ni-base (solid sol.) | 1354                          | 760.1                       | 1.639e-04 | 10       | 0.22850 | 4,314  |
| 19  | Ti6AlV | α and β phases | 1604                          | 501.6                       | 1.791e-04 | 134      | 0.01299 | 12 367 |
| 20  | Haynes 355 | Fe-Ni-base (solid sol.) | 1371                          | 775.6                       | 1.039e-04 | 1390     | 0.00107 | 3,771  |
| 21  | Haynes 230 (a) | Ni-base (solid sol.) | 1288                          | 798.4                       | 0.002124   | 1591     | 0.00376 | 6,176  |
| 22  | Haynes 230 (b) | Ni-base (solid sol.) | 1288                          | 829.3                       | 0.002035   | 260      | 0.12314 | 7,681  |
| 23  | Haynes 188 | Co-base (solid sol.) | 1315                          | 932.8                       | 0.001307   | 4807     | 0.00138 | 6,002  |
| 24  | Hastelloy C22 | Ni-base (solid sol.) | 1357                          | Not enough high-temp data pts. |                       |                      | 0.00020 | 4,647  |
| 25  | Hastelloy S | Ni-base (solid sol.) | 1335                          | 765.2                       | 8.509e-05 | 454      | 0.00859 | 6,211  |
| 26  | Hastelloy X | Ni-base (solid sol.) | 1260                          | 837.6                       | 0.002745   | 212      | 0.13881 | 5,298  |
| 27  | Hastelloy X (10 μm) | Ni-base (solid sol.) | 1260                          | 744.4                       | 0.003165   | 137      | 0.24225 | 11 620 |
| 28  | Rene 95 | Ni-base (precipit. hard.) | 1343                          | 627.6                       | 0.000001   | 80 757   | 0.00135 | 217 771|
| 29  | Rene 41 | Ni-base (precipit. hard.) | 1316                          | 748.1                       | 0.000009   | 663      | 0.03624 | 79 716 |
| 30  | Pure Nickel | Ni-base | 1455                          | Not enough high-temp data pts. |                       |                      | 0.00892 | 64      |
| 31  | Nickel 201 | Ni-base (solid sol.) | 1435                          | Not enough high-temp data pts. |                       |                      | 0.00246 | 132     |
| 32  | Nickel 200 | Ni-base (solid sol.) | 1435                          | 349.4                       | 0.001337   | 22       | 0.01677 | 258     |
| 33  | Nimonic 263 | Ni-base (precipit. hard.) | 1300                          | 758.8                       | 0.000262   | 82       | 0.08506 | 15 601 |
| 34  | Nimonic 90 | Ni-base (precipit. hard.) | 1310                          | 724.8                       | 7.875e-05 | 74       | 0.08111 | 29 514 |
| 35  | Nimonic 80a | Ni-base (precipit. hard.) | 1320                          | 754.3                       | 0.000351   | 156      | 0.05091 | 19 933 |
| 36  | Nimonic 75 | Fe-Ni-base (solid sol.) | 1340                          | 731.2                       | 0.001561   | 92       | 0.06840 | 1,391  |
| 37  | Nimonic PE16 | Fe-Ni-base (precipit. hard.) | 1310                          | 731.6                       | 2.512e-05 | 7        | 0.1399  | 16 557 |
| 38  | Nimonic PE13 | Fe-Ni-base (solid sol.) | 1310                          | Not enough high-temp data pts. |                       |                      | 0.00131 | 6,424  |
| 39  | N155 | Fe-Ni-base (solid sol.) | 1288                          | 847.5                       | 0.008876   | 687      | 0.0670  | 2,998  |
| 40  | L605 | Co-base (solid sol.) | 1330                          | Not enough high-temp data pts. |                       |                      | 0.00782 | 3,666  |

Average (No. 1-2, 4-9, 11, 14-23, 25-30, 32-37, and 39): 0.00175 4151 0.0525 25 836
low-temperature regime. Automated black-box model ML suites, such as the Tree-Based Pipeline Optimization Tool, may be inappropriate due to their limited ability to provide much-needed insights into the underlying physics. Instead, one is motivated to make the most of the limited data available by incorporating important a priori information about the underlying physics into the model structure, for the purpose of deriving such insights. Specifics on the algorithmic aspects of the incorporation of a priori information into the bilinear log model are presented in Section 4. The results in Figure 2–4 were derived using the global-optimization approach, applied separately to individual alloys, for the purpose of obtaining a tighter fit and more accurate estimation of $T_{break}$ than for separate optimization over the low- and high-temperature regimes.

In regards to the underlying physics, Ni-based superalloys containing $\gamma'$ phases tend to be particularly resistant to temperature with reference to their in-service mechanical properties. Strengthening generally occurs through both alloying elements acting as solutes in the face-centered-cubic (FCC) austenitic matrix phase and through the solute-precipitation strengthening, such as the $\gamma'$ phase. This phase is responsible for the YS of many nickel-based superalloys being relatively insensitive to temperature. The effect arises from dislocation locking on secondary slip planes caused by cross-slipping of primary dislocations on $\{111\}$ slip planes in the $\gamma'$ phases during plastic deformation. Ordinary dislocation slip occurs on the $\{111\}<110>$ plane, both for the $\gamma$ and the $\gamma'$ phases. There is, however, a tendency for dislocations in the $\gamma'$ phase to cross-slip onto secondary $\{100\}$
planes, where they can have a lower anti-phase domain boundary energy (APB). These secondary slip planes are thermally activated, similar to the APB energy, which is crucial for maximizing the strengthening provided by the presence of $\gamma'$ phases. At the same time, strengthening contributions from both the $\gamma'$ phase and the APB energy decrease with an increase in temperature. This correlates with findings in the present results, such as the signature peak in the flow stress, seen for $\gamma'$-strengthened superalloys.

When higher strength is required at lower temperatures, e.g., for turbine discs, precipitation strengthening in Ni-based superalloys can still be utilized, either by employing other phases, such as the $\gamma''$ phase in Nb-bearing alloys or multimodal size distribution of the $\gamma'$ phase. The $\gamma''$ phase occurs in Ni-based superalloys, such as Inconel 718, which have significant addition of Niobium or Vanadium. The stoichiometry of the $\gamma''$ phase is $\text{Ni}_3\text{Nb}$ or $\text{Ni}_3\text{V}$ and consists of a body-centered-tetragonal lattice with an ordered arrangement of Nickel and Niobium atoms. Strengthening occurs primarily through coherency-hardening and order-hardening mechanisms.

The governing deformation mechanism is ordinary slip on the $\{111\}<110>$ plane, both for the $\gamma$ and the $\gamma'$ phases. There is, however, a tendency for dislocations in the $\gamma'$ phase to cross-slip onto $\{100\}$ planes, where they can attain a lower APB energy. Situations can arise where an extended dislocation is partly on a close-packed plane and partly on a cube plane. Such a dislocation can become locked and result in an increase in strength, which can help retain strength in the low-temperature regime. In the elevated-temperature regime, thermally activated microstructural phenomena tend to be sufficiently violent to allow dislocations to overcome obstacles.

**Figure 4.** Quantification of modeling accuracy of the bilinear log model for the composition No. 27 from Table 1 (Hastelloy X 10 μm), and comparison to that of a model with a single exponential, a) in the logarithmic domain and b) in the linear domain.

**Figure 5.** Comparison of temperature-dependent YSs across superalloy compositions. The three primary categories of superalloys are commonly identified in the literature as...
1) Fe-Ni, 2) Ni-, and 3) Co-based superalloys.[1] Fe-Ni-based superalloys, such as the popular Inconel 718, came into existence as an extension of the stainless-steel technology and are generally heat treated for both their wrought and cast conventions. Co- and Ni-based superalloys may be heat treated or not, wrought or cast, depending on the application and composition involved. Figure 5 illustrates the following: 1) The precipitation-strengthened superalloys seem to result in higher YS than the solid-solution-strengthened ones in the case of both the Ni-based and the Fe-Ni-based superalloys. 2) The Ni-based superalloys tend to produce higher YS than the Fe-Ni-based superalloys in the case of both precipitation and solid-solution strengthening.

The superior YS of the precipitation-strengthened superalloys is illustrated in Figure 5, reproduced from strength-temperature diagrams widely utilized in the literature.[1] Superalloys can be strengthened not only through solid-solution strengthening but also through the presence of strengthening phases, such as precipitates. Co-based superalloys can exhibit a tendency toward the transformation of the FCC matrix phase into stable lower temperature phases. In the case of Ni- and Fe-Ni-based superalloys, the FCC matrices can exhibit favorable characteristics for the precipitation of uniquely effective strengthening phases.[1]

When looking at the superalloy compositions from the Supporting Information, the following observations stand out: 1) Many of the superalloys, such as Astroloy, Hastelloy S, Hastelloy X, and Waspaloy, Nimonic PE16, Rene 41, Nimonic 80a, Nimonic 90, Rene 95, Nickel 200, Nimonic 263, Udiment 520, Udiment 500, Haynes 556, Inconel 600, Inconel 601, Incoloy 825, and Inconel 807, present fairly straightforward low- and high-temperature regimes.

A flat intermediate regime, such as observed for Udiment D979, Inconel 802, Inconel 800, Inconel 625, Inconel 617 (sheet), Haynes 188, and Nimonic 75, has also been reported for medium- and high-entropy alloys (MEAs and HEAs) in prior work by Steingrimsson et al.[13] These cases may necessitate the application of the tri-linear log model from Equation (13)–(16). Possible explanations for a tri-linear behavior for intrinsic temperature-dependent YSs in body-centered cubic (BCC) metals and substitutional solid solutions have been discussed by some researchers:[14] 1) Plastic deformation of the BCC metals and alloys is believed to be mediated by the thermally activated formation and movement of kink pairs at low temperatures. 2) Above a certain “critical temperature”, a flat-strength plateau is achieved, where the strength becomes virtually temperature or strain-rate independent. 3) When the test temperature exceeds approx. 40% of the melting temperature, diffusional processes can lead to a rapid decrease of yield stress, and the YS becomes strain-rate dependent again.

In the presently utilized case of the tri-linear log model, two break temperatures, \( T_{break1} \) and \( T_{break2} \), are considered.[3] However, the explanations outlined previously only reference one such temperature and refer to it as the “critical temperature” or “knee temperature”, which apparently corresponds to \( T_{break1} \) in our model.

The flat intermediate plateau seems less prevalent in alloys with FCC-crystal structures. The FCC-crystal structure possesses 12 slip planes with 4 closest packed \{111\} planes and 3 closest packed \{110\} directions per plane. The hexagonal close packed (HCP) crystal structure, on the other hand, only has three active slip systems at room temperature. The BCC crystal structure does not have truly closest packed planes, but one closest-packed direction, the \{111\} direction; therefore, dislocation mobility is critically dependent on thermal activation in BCC metals.

Extensive research has been conducted on the subject of slip systems, Peierls barriers, dislocation mechanisms, flow stress, and temperature-dependent stress behavior in BCC vs FCC metals; see, for example, works by Seeger et al.[15,16] In the specific case of Inconel 718, the need for a tri-linear log model may be hard to ascertain due to the possible uncertainty in the experimentally measured data points.

The hump between the low- and high-temperature regimes, i.e., the anomalous yield-strength phenomenon, is characteristic of the \( \gamma' \) - or \( \gamma'' \)-strengthened superalloys.[3,12] The phenomenon manifests itself as a positive temperature dependence of the total YS and is found in superalloys strengthened by L1_2-ordered intermetallics.[17] The increasing strength of the \( \gamma' \) phase with temperature is explained by a thermally-activated cross slip of dislocations from \{111\} planes to \{100\} planes, where locking of partial dislocations occurs.[18,19] The influence of the \( \gamma' \) strengthening increases with increasing \( \gamma' \) volume fraction and increasing temperature below the peak YS, as seen in Figure S5 from the Supporting Information.[11,20] Additional factors involve the \( \gamma' \) size, \( \gamma' \) solute content, \( \gamma'-\gamma \) mismatch, and both the stacking fault energy as well as the APB energy. The latter two factors are the major contributions to hardening for both the matrix phase as well as the precipitate phase and are both strongly affected by alloying additions.[23]

Supplementary datasets for the factors mentioned above were collected for all the alloys presented in Table S1 from the
3. Conclusions

In conclusion, we proposed a bilinear log model for predicting the YS of superalloys across temperatures and studied its effectiveness for 38 distinct compositions or 40 total configurations. We considered the break temperature, $T_{\text{break}}$, an important parameter for the design of superalloy materials with favorable properties at elevated temperatures, one warranting the inclusion in the superalloy alloy specifications. For reliable operations, and not accounting for coatings, the operating temperatures for the corresponding superalloys may need to stay below $T_{\text{break}}$. Earlier models for the temperature dependence of the YS only accounted for a single exponential and thus did not feature a break temperature. Across these 40 configurations, we demonstrated a much superior performance of the bilinear log model compared to the one comprising a single exponential. In the logarithmic domain, the bilinear log model resulted in MSE of 0.00175, compared to the MSE of 0.0525 for the single-exponent model. But in the linear domain, the bilinear log model produced MSE of 4151 MPa$^2$, averaged across these 40 configurations, compared to the MSE of 25 836 MPa$^2$ for the single-exponent model. Our observations regarding the superior YS behavior of precipitation-strengthened superalloys, compared to solid-solution strengthened superalloys, for both the Ni- and Fe-Ni-based superalloys, were consistent with literature data.$[^3]$ Similarly, our observations concerning superior YS properties of Ni-based superalloys, compared to Fe-Ni-based superalloys, in the case of both precipitation and solid-solution hardening, were also consistent with the available literature.$[^5]$

4. Experimental Section

Although the primary emphasis here is on the YS, the optimization of the mechanical properties is assumed to take place within a framework for joint optimization.$[^6,13]$

Methodology for Maximization of the YS: Our approach accurately captures the input sources that contribute to variations in the YS observed relative to variations in the output. The input parameters for the model used in the present work are:

$$\text{Input} = (\text{composition, } T, \text{ process, defects, grain size, microstructure})$$

In this context, “defects” are defined broadly, such as to include inhomogeneities, impurities, dislocations, or other microstructural features, while $T$ represents temperature. Analogously, the term “microstructure” broadly represents microstructures here, at the nano or the microscale, as well as phase properties, and the term “process” broadly refers to manufacturing processes and any type of postprocessing. Similarly, the term “grain size” generally refers to the size distribution of all grains.

Table S1 from the Supporting Information, comprises an initial step toward parametrization of the microstructure of the superalloys under study. Table S1 from the Supporting Information, lists key microstructure properties that impact the high-temperature strength properties of the superalloys at hand. According to Table S1 from the Supporting Information, these microstructure properties involve the precipitate/dispersoid type, the volume fraction, the average grain size of the primary precipitate, the average grain size of the secondary or aged precipitate form, the grain size of the matrix, as well as the lattice mismatch between the austenite matrix and precipitate phase at a constant temperature. In our modeling, we seek to focus on the influence of a specific microstructural feature, secondary strengthening phases, such as $\gamma'$, as identified by the existence of inflection (break) points in our modeling results. Section 4.4 of ref. [4] addresses the expected dependence of the US on the individual input sources listed. The prediction model can be summarized as:

$$\text{US} = h[\text{composition, } T, \text{ process, defects}(\text{process, } T), \text{grains}(\text{process, } T), \text{microstructure}(\text{process, } T)]$$

If the YS corresponding to a certain input combination is known, one can simply look up the known value. However, if the YS corresponding to a given input combination is not known, then a prediction step can be applied (e.g., interpolation or extrapolation).$[^{13}]$

Methodology for Modeling YS at Elevated Temperatures: Senkov et al. provide physics-based foundation for the bilinear log model.$[^9]$ The diffusion processes required to initiate phase transformations generally become noticeable at temperatures $T > 0.4 T_m$, according to Senkov et al., while at $T < 0.4 T_m$ the phase transformations are kinetically restricted.$[^{10}]$ When $T < 0.4 T_m$, the atoms are generally not able to move out of the lattice, and no phase transformations can take place. This tendency applies to low-entropy alloys, MEAs, and HEAs and serves to explain a model comprising two exponentials.$[^9]$ A single-exponential model does not take into account diffusion effects and agrees well with the experimental data only at relatively low temperatures, where diffusion-controlling deformation mechanisms can be ignored. But as the temperature increases, the chemical bonds between the elements become softer. A diffusion-controlled regime is generally observed above $\approx 0.5$–$0.6 T_m$. The diffusion-controlled regime can be distinguished from the low-temperature regime by a more rapid drop in strength with increasing temperature because now dislocations are able to move more easily around obstacles.$[^{11}]$

Motivated by Figure 3c,d of ref. [3], along with the physics-based insights from ref. [6], we model the temperature dependence of the YS($T$), in terms of a bilinear log model, parametrized by the melting temperature, $T_m$, as follows:$[^{13}]$

$$YS(T) = \min(\log(YS_1(T)), \log(YS_2(T)))$$

$$YS_1(T) = \exp(-C_1 \times T/T_m + C_2), \quad 0 < T < T_{\text{break}}$$

$$YS_2(T) = \exp(-C_3 \times T/T_m + C_4), \quad T_{\text{break}} < T < T_m$$

$$T_{\text{break}} \text{ is subject to a separate physics (diffusion)-induced constraint}$$

$$0.33 \leq T_{\text{break}}/T_m \leq 0.55$$
As elucidated in[13] a conceptually simple approach for fitting the model in Equation (5)–(10) to the YS data available consists of first deriving the constant coefficients, $C_1$ and $C_2$, by applying linear regression to the data points available to the lowest temperature region ($0 < T < 0.35 T_m$) as well as to the intermediate region ($0.35 T_m < T < 0.55 T_m$). One can then obtain the constants, $C_3$ and $C_4$, by applying linear regression to the data points available to the intermediate ($0.35 T_m < T < 0.55 T_m$) and high-temperature ($T > 0.55 T_m$) regions. Note that $T_{break}$ does not have to be known in advance. As supported by Equation (10), $T_{break}$ is an inherent property of a given alloy that emerges from the model as the break point between the two linear regions. The model in Equation (5)–(7) comprises only four independent parameters, $C_1$, $C_2$, $C_3$, and $C_4$, which simply can be estimated by applying linear regression separately to low- and high-temperature regimes, even to a fairly small data set. Note, furthermore, that for a new alloy system, linear regression needed) and a trilinear log model (a possibly nonconvex algorithm based on the MATLAB pseudo-code in Supplementary Figure 7 of ref. [3] for the bilinear log model, four data points are needed for the full definition of the problem (since the bilinear log model contains four parameters). Similarly, for concurrent optimization over the individual-temperature regimes, using an algorithm based on the MATLAB pseudo-code in Supplementary Figure 8 of ref. [3] for the trilinear log model, eight data points are needed for full definition of the problem (since the model now contains eight parameters). Table S2 and S3 from the Supporting Information, illustrate that large majority of the superalloy compositions under consideration comprise of fewer than eight $(T_{YS})$ combinations.

As for the black-box models, it is important to consider the small number of YS($T$) data points for a given superalloy composition, per Table S2 and S3 from the Supporting Information. With typically only 5–7 YS($T$) combinations measured for most superalloy compositions, excluding the one corresponding to no YS at the solvus temperature, black-box models may be limited to a single layer and several nodes (assuming at least one input data point per model parameter to be estimated). The small size of the data set does not allow for separate training and testing sets. The small size of the data set, for each superalloy composition, in this case, does not allow for meaningful implementation of black-box models. Hence, to make the most of the limited data set available, it is important to consider the physics-based modeling of the YS.

Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.

Acknowledgements

X.F. and P.K.L. very much appreciate the support of the U.S. Army Research Office Project (W911NF-13-1-0438 and W911NF-19-2-0049) with the program managers, Drs. M. P. Bakas, S. N. Mathaudhu, and D. M. Stepp. P.K.L. thanks the support from the National Science Foundation (DMR-1611180, 1809640, and 2226508) with the program directors, Drs. J. Madison, J. Yang, G. Shifer, and D. Farkas. X.F. and P.K.L. also appreciate the support from the Bunch Fellowship. X.F. and P.K.L. would like to acknowledge funding from the State of Tennessee and Tennessee Higher Education Commission (THEC) through their support of the Center for Materials Processing (CMP). BS very much appreciates the support from the National Science Foundation (IIP-1447395 and IIP-1632408), with the program directors, Drs. G. Larsen and R. Mehta, from the U.S. Air Force (FA864921P0754), with J. Evans as the program manager, and from the U.S. Navy (N6833521C0420), with Drs. D. Shifer and J. Wolk as the program managers. The authors also want to thank Dr. Graham Tewksbury for offering insightful comments on strengthening mechanisms in superalloys during an October 21, 2021, material science graduate seminar presentation, conducted by BS at Oregon State University. The authors similarly want to thank Dr. Chanho Lee for bringing precursors to Figure S1–S3 from the Supporting Information, to their attention.

Conflict of Interest

The authors declare no conflict of interest.
Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Keywords

high temperature, machine learning, physics-based modeling, structural materials, superalloys, yield strength

Received: December 28, 2022
Revised: February 27, 2023
Published online: March 23, 2023

[1] M. J. Donachie, S. J. Donachie, in Superalloys, A Technical Guide 2nd edition, ASM International, Almere, The Netherlands 2002.
[2] B. Steingrimsson, X. Fan, A. Kulkarni, D. Kim, P. K. Liaw, US Patent 16/782,829, 2020.
[3] B. Steingrimsson, X. Fan, X. Yang, M. C. Gao, Y. Zhang, P. K. Liaw, NPJ Computational Materials 2021, 7.
[4] B. Steingrimsson, X. Fan, A. Kulkarni, M. C. Gao, P. K. Liaw, in High-Entropy Materials: Theory, Experiments, and Applications, (Eds: J. Brechtl, P. K. Liaw), Springer Nature, Cham, Switzerland 2021, pp. 115–238.
[5] A. Agrawal, P. D. Deshpande, A. Cecen, G. P. Basavarsu, Integrat. Mater. Manuf. Innov. 2014, 3, 90.
[6] O. N. Senkov, S. Gorsse, D. B. Miracle, Acta Mater. 2019, 175, 394.
[7] Z. Wu, H. Bei, G. M. Pharr, E. P. George, Acta Mater. 2014, 81, 428.
[8] F. Maresca, W. A. Curtin, Acta Mater. 2020, 182, 235.
[9] H. K. D. H. Bhadeshia, in Nickel Based Superalloys, University of Cambridge, Cambridge, UK 2019.
[10] T. T. Le, W. Fu, J. H. Moore, Bioinformatics 2020, 36, 250.
[11] R. C. Reed, in The Superalloys: Fundamentals and Applications, Cambridge University Press, Cambridge, UK 2008.
[12] C. T. Sims, N. S. Stoloff, W. C. Hagel, Superalloys II, Vol. 8. Wiley, New York 1987.
[13] B. Steingrimsson, X. Fan, R. Feng, P. K. Liaw, Appl. Mater. Today 2023, 31, 101747.
[14] H. Chen, A. Kauffmann, S. Laube, I. C. Choi, R. Schwaiger, Y. Huang, K. Lichtenberg, F. Muller, B. Gorr, H. J. Christ, M. Heilmayer, Metall. Mater. Trans. A 2018, 49, 772.
[15] A. Seeger, Mater. Sci. Eng. A 2001, 319–321, 254.
[16] A. Seeger, Zeitschrift für Metallkunde 2002, 93, 760.
[17] A. Sengupta, S. K. Putatunda, L. Bartosiewicz, et al., J. Mater. Eng. Perform. 1994, 3, 73.
[18] B. Kear, Trans. Metall. Soc. AIME 1962, 224, 674.
[19] B. Kear, Trans. Metall. Soc. AIME 1962, 224, 669.
[20] T. Kruml, E. Conforto, B. Lo Piccolo, D. Caillard, J. L. Martin, Acta Mater. 2002, 50, 5091.
[21] Z. Chen, K. Kishida, H. Inui, M. Heilmayer, U. Glatzel, G. Eggeler, Acta Mater. 2013, 238, 118224.
[22] E. I. Galindo-Nava, C. M. F. Rae, Mater. Sci. Eng. A 2015, 636, 434.
[23] E. I. Galindo-Nava, L. D. Connor, C. M. F. Rae, Acta Mater. 2015, 98, 377.
[24] F. Otto, A. Diouhy, C. Somsen, H. Bei, G. Eggeler, E. P. George, Acta Mater. 2013, 61, 5743.