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Article

Developing a neural network to model the mechanical properties of 13-8 PH stainless steel alloy

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SUMMARY
We systematically evaluated the effects of raw material composition, heat treatment, and mechanical properties on 13-8PH stainless steel alloy. 13-8PH is widely used in the aerospace industry for various structural components. Little is known about the predictive modeling of mechanical properties for 13-8 PH per heat treatment. To achieve the desired properties, multiple back-and-forth heat treatments and mechanical tests are often required which utilize significant amounts of resources. Thus, we hypothesized that no specific heat treatment temperature can be used to achieve the desired property ranges across all 13-8PH compositions. We heat treated 13-8PH alloy through solution treatment, cryogenic treatment, and final elevated temperature aging. We conducted double shear testing to measure this mechanical property. Consistent with expectations, experimental data confirmed that no single specific aging heat treatment temperature could be used to achieve desired property range for all compositions. A unique aging heat treatment temperature is required and there is a need to develop a model to predict heat treatment response for each composition. The results of the neural network models were in agreement with our experimental results and aided in the evaluation of the effects of aging temperature on double shear strength. The data suggests that this model can be used to determine the appropriate 13-8PH alloy aging temperature needed to achieve the desired mechanical properties, eliminating the need for many costly trials and errors through re-heat treatments.

INTRODUCTION
13-8PH is a precipitation-hardening stainless steel. It has a versatile combination of high strength, good ductility, toughness, and weldability (1–3). Because it also has high resistance to general corrosion and stress corrosion cracking, 13-8PH is more suitable for structural critical applications compared to other precipitation-hardened stainless steels such as 17-4PH or 15-5PH (1–3). Thus, this alloy is currently widely used for various aerospace and industrial applications, including gears, fasteners, fittings, shafts, and turbine blades. Also, due to its high ductility, this alloy can be fabricated into different shapes and forms, such as bars, wires, and forgings.

The typical route for manufacturing aerospace structural components starts with forging, machining, and heat treatment. This is followed by in-process testing and additional forming operations, then non-destructive testing and surface engineering such as coatings. The manufacturing is then finalized by completing final testing and inspections. Heat treatment is used in metalworking to reach the desired properties of strength, malleability, and resistance (4). For 13-8PH, applying proper heat treatment can result in a wide range of shear strength and ductility (1). To achieve the optimal strength and ductility combinations for 13-8PH alloy, special heat treatment processing must be used via governing specification 23M112 (4). The 23M112 specification covers the requirements for high strength 13-8PH components which ensure quality and safety. Per 23M112 specification, the heat treatment processing starts with the raw material 13-8PH being solution treated at 926°C for one hour, then it undergoes cryogenic treatment at -73°C for at least 2 hours, and finally it undergoes an additional elevated temperature aging of between 510–538°C for 4 hours (1, 5). The final aging temperature is adjusted to maximize the ductility while maintaining a minimum shear strength of 862-952 MPa. This results in a good combination of strength and ductility (5). Within the industry, it would be ideal to use the same heat treatment processing parameters for all raw material 13-8PH compositions to achieve identical properties. However, multiple back-and-forth heat treatments and mechanical tests are often required to guarantee the desired properties which utilizes significant resources. With recent developments in computer technology, predictive heat treatment models for some aerospace alloys have emerged that can accurately predict properties without the need for wasteful extra heat treatment and testing.

Mathematical modeling and simulation have increased in value as industrial tools, with considerable progress having been achieved in this research field within the last decade (6). Some specific areas where mathematical modeling has been useful include the use of neural networks to identify and calculate the mathematical correlation between metal properties and heat treatment, temperature-phase transformation-stress, and phase transformation kinetics (7, 8). All these achievements have provided a sound basis for applying computer simulation technology to practical manufacturing property prediction. The performance of a neural network model depends on the quality of the dataset used for its training. Neural networks are typically adopted due to the non-linear nature of the dataset given to it and their ability to recognize relationships between data using training algorithms (6, 9). Typically, a standard feed-forward network with one input layer, one hidden layer, and one output layer is used. Each layer consists of units, or neurons. In each layer, units received their input from the preceding layer's units and would then send their output to units in the subsequent layer.

From raw materials to finished processing, the final properties of 13-8PH are always influenced by the process parameters. Thus, understanding and developing a predictive model that could report strong correlations between processing parameters and mechanical properties is valuable and an industrial objective. Developing a thorough understanding of these process parameters, such as heat treatment processing temperature, will provide valuable methods for producing complex and high-quality aerospace components.

To our knowledge, little is known about the exact relationships between raw 13-8PH alloy composition and mechanical properties, heat treatment temperatures, and strength. The industry heavily relies on extensive mechanical testing to verify such properties (4, 5). In addition, no statistical model is available to predict the effects of heat treatment temperature on 13-8PH strength.

Therefore, we hypothesized that no single specific heat treatment temperature can be used to achieve the desired property range across all 13-8PH compositions per current governing specification 23M112 (5). We completed a detailed characterization of the impact of heat treatment temperature on double shear strength. We expected that a unique heat treatment temperature would be required for each composition. Then, we aimed to develop a predictive model that would accurately corroborate the experimental data. Thus, a model was built for the modeling, statistical analysis, and optimization of the processing parameters and properties. Specifically, the present work attempts to establish the relationship between the aging heat treatment temperature, raw material composition and properties, and the final mechanical properties of 13-8PH alloy. Our results indicated that a neural network predictive model can be developed to predict aerospace alloy 13-8PH heat treatment response with high accuracy. In addition, this predictive modeling approach can be developed to incorporate many other aerospace and industrial materials heat treatment and processing.

RESULTS

Heat treatment response of various compositions of 13-8PH

We aimed to systematically evaluate the effect of heat treatment on 13-8PH properties via double shear testing. To evaluate our hypothesis, we randomly chose three compositions: A, B, and C (**Table 1**). For this experiment, all three compositions underwent the same solution, cryogenic, and aging treatment. However, the final aging temperature was different across all three compositions in this experiment. As expected, the measured shear strength dropped with an increasing aging temperature. However, a different heat treatment response was identified for each composition. To represent the acceptable aging treatment temperature of 510–538°C and double shear strength within the 862-952 MPa ranges required by the 23M112 specification, a dotted black box was drawn (**Figure 1**). Any data point outside the dotted black box was not acceptable as it violated specification 23M112 and would have either resulted in an unacceptable double shear strength and/or an unacceptable heat treatment temperature.

Table 1. Compositions used to evaluate heat treatment response

13-8PH Alloy	Elemental Composition (%)									
	C	Mn	Si	P	S	Cr	Ni	Mo	Al	N
A	0.030	0.004	0.07	0.005	0.002	12.54	8.08	2.11	1.08	0.004
B	0.031	0.04	0.03	0.007	0.0007	12.48	8.24	2.21	1.01	0.0031
C	0.040	0.02	0.06	0.005	0.002	12.59	8.18	2.09	1.1	0.004

For composition A of 13-8PH alloy, the full range of the aging temperatures between 510–538°C can be used while still meeting the strength requirements of 862-952 MPa because none of the data extends outside the solid black box. In other words, the 23M112 specification's required range of double shear strength 862-952 MPa can be obtained by using the required aging temperature treatment range of 510–538°C (**Figure 1**). However, this did not apply for compositions B and C. The 23M112 specification required range of double shear strength 862-952 MPa cannot be obtained using the specification required aging temperature treatment range of 510–538°C. For composition B, any aging temperature between 529–538°C could lead to excessively

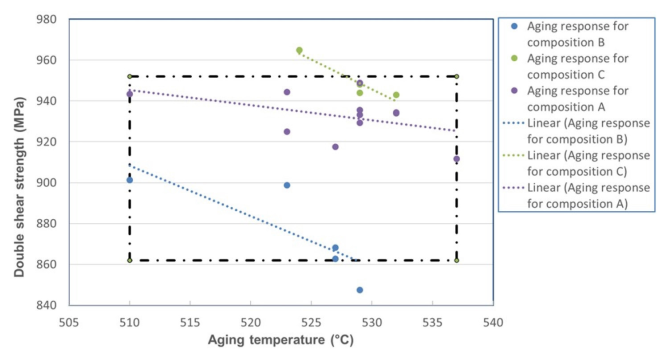

Figure 1. Relationship between aging temperature and double shear strength for three compositions of 13-8PH alloy. All three composition materials underwent the same solution treatment at 926°C for 1 hour, followed by cryogenic treatment at -73°C for 2 hours. Following mechanical double shear testing, the final aging process was conducted between 510–538°C for 4 hours. n = 5 is applied for each processing temperature with only the average displayed. The dotted line represents the linear regression trend line between double shear strength and aging temperature. The dotted black box represents the required aging temperature and property ranges per specification 23M112 (4).

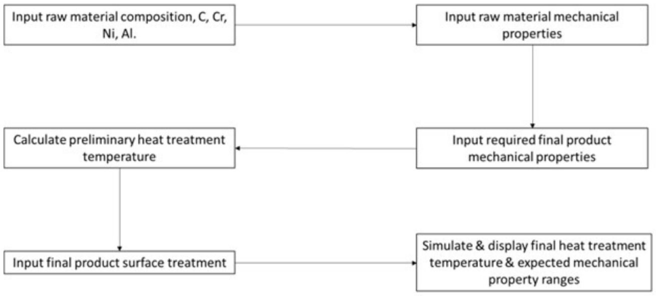

Figure 2. Statistical flow chart for 13-8PH mathematical model. The workflow of the processing model used to simulate the effects of raw material composition and properties, and aging temperature on double shear strength of various 13-8PH alloy compositions.

lower shear strengths than the required 862 MPa. This violates specification 23M112 as indicated by the data located below the solid black box which means that its double shear strength is lower than the 23M112 required double shear strength (**Figure 1**) (5). Similarly, for composition C, any aging temperature between 510–529°C could lead to excessively higher shear strengths than the required strength of 952 MPa. This also violates specification 23M112 as indicated by the data located above the solid black box which means that the strength is higher than the 23M112 required double shear strength (**Figure 1**) (4). Thus, this clearly indicated the different heat treatment responses for different raw material 13-8PH alloy compositions. Our data therefore suggested that it would have been impossible to use the same heat temperature processing parameters to achieve identical properties across all raw material compositions since different heat treatment responses were identified via the current governing specifications.

Statistical modeling

Our heat treatment response results indicated the need to be able to precisely predict the aging heat treatment response based on incoming 13-8PH conditions such as composition and property. To achieve this, a flow chart was designed to represent the steps and sequences of workflow to develop the heat treatment strength prediction model (**Figure 2**). Within the flowchart, a statistical model was created to simulate the effect of 13-8PH alloy composition and aging temperature on the shear strength of each alloy.

To validate the statistical model, a new set of experiments was conducted and compared to the model. An additional raw material, composition D, which was not part of the data to build the model was randomly chosen (**Table 2**). As before, the same solution and cryogenic treatment were conducted, while only the final aging temperature was altered. As

Table 2. Composition used for verifying heat treatment model.

13-8PH Alloy	Elemental Composition (%)									
	C	Mn	Si	P	S	Cr	Ni	Mo	Al	N
D	0.031	0.04	0.03	0.007	7E-04	12.48	8.24	2.21	1.01	0.0031

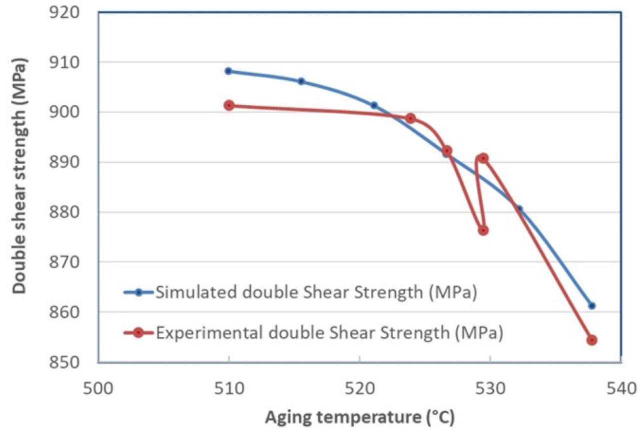

Figure 3. Predicted versus experimental shear strength across a range of aging temperatures for composition D. To validate the model, an additional raw material, composition D underwent the same solution at 926°C for 1 hour, followed by cryogenic treatment at -73°C for 2 hours. Following mechanical double shear testing, final aging was conducted between 510–538°C for 4 hours. Blue line represents simulated strength values made by the model based on composition D. Red line represents the experimental strength data.

expected, a higher aging temperature predicted a lower strength in the material (**Figure 3**). An ANOVA and Tukey's post hoc test were used to evaluate the statistical significance of pairwise differences between means of simulated and experimental shear strength (10). The calculated Tukey 95% confidence interval showed that the mean shear strength difference between the simulated and experimental data was not statistically significant because the interval contained zero. In addition, the model showed an R^2 of 0.8, the coefficient of determination, indicating that the experimental data was in good alignment with the simulated data. Thus, we successfully demonstrated that a model with experimental data in good alignment with simulated data could be achieved.

DISCUSSION

The goal of this study was to systematically evaluate the effect of raw material composition, raw material properties, and aging temperature on double shear strength through experiments and statistical modeling. Consistent with expectations and the hypotheses, no single specific heat treatment temperature could be used to achieve desired property range for all compositions using existing governing specification 23M112 (5). Thus, within the industry, only a limited range of aging temperatures can be used to meet industry specification 23M112 (5). Furthermore, the aging temperature range must be specific and likely narrowed with reduced ranges for each unique composition. Part of the reason for this could potentially be that there are raw material variations depending on the suppliers. These variations can include variability in composition and other properties. Because of the variability, the resulting heat-treated strength is expected to be different for different compositions. Without predictive modeling, either a repeat of the entire cycle of heat treatment from resolution and re-cryogenic treatment to re-aging or a shortened re-aging treatment is required to achieve the desired properties range. In general, re-heat treatment should be avoided because the end material properties are even more difficult to predict, and the process is costly in both time and resources.

Consistent with expectations, a statistically reliable model was developed which achieved an R^2 of 0.8 along with experimental verifications indicating the model could be used to reliably predict the final mechanical properties of 13-8PH alloy with a given heat treatment. This model provided a strong foundation for the ability to predict aging temperature, which suggests that it can be used to replace the previously used method of randomly guessing while also being able to potentially allow for significant cost savings. Furthermore, this predictive modeling approach can be extended to many other alloys such as 15-5PH which is widely used in the aerospace industry and requires even tighter property ranges of up to only ±2% double shear strength (11). To achieve optimal strength, ductility, and corrosion resistance, it would be ideal to have well-specified strength and ductility ranges. Considering the variability of raw material composition and heat treatment responses, developing a predictive model that can accommodate these variations should lead to optimal properties with lower costs and without needing to conduct costly random guesses of heat treatment temperatures.

Nevertheless, further studies are required to improve the model. With an R^2 of 0.8, 20% of the property variations still cannot be explained by this model. This could be because the current model did not incorporate all potential variables. One missing variable could be the compositional variation within the same batches of raw material. It is typical to have composition variation across the whole wire and bar. Another missing variable could be variation in the double shear testing. It is well known that double shear testing data depends on the intrinsic material strength, as well as other testing variables such as surface friction coefficient and fixtures (12). In measured double shear strength, the surface friction can lead to variation of up to 4%. Thirdly, the sample size might not be comprehensive enough to cover all variants of the composition. This could also potentially affect the model. Finally, there might be some other important material and processing characteristics that were not incorporated into this model such as microstructural features, solution aging temperature, cryogenic aging temperature, and aging temperature profile variations. Therefore, future studies shall incorporate more variables to further improve predictability. Moving forward, this statistical model approach can be improved and extended to other aerospace alloys with significant cost savings and lead to time reductions.

MATERIALS AND METHODS

13-8PH raw material

All the materials and data were supplied by Avantus Aerospace (Compton, CA). Different batches of 13-8PH alloy per material specification AMS5629, in the form of bar or wire, were obtained (13). The diameters of the bars and wires ranged from 4.2 to 12.8 mm. The geometry differences within the incoming materials were not expected to have any real impact on the results since high-temperature solution treatment at 926°C for one hour should have been able to eliminate all prior processing differences.

Heat treatments

Standard solution heat treatment per specification 23M112 was conducted at 926°C for 1 hour, which was then followed by an air-cool process to -73°C for 2 hours within 24 hours after solution treatment (5). Final precipitating age hardening was completed between 510–538°C for 4 hours following the air cool process per 23M112 specifications. The final precipitating age hardening temperature was adjusted to meet the double shear strength range of 862–952 MPa per 23M112 (5). During this evaluation, solution and cryogenic treatment were the same across all conditions, and only the final aging temperature was adjusted to meet the desired shear strength (862–952 MPa). In total, 251 data sets from Avantus were used for this simulation.

Mechanical testing

Double shear testing was conducted per aerospace standard NASM1312-13 (14). A hardened steel blade was used for double shear testing by accurately cutting out the diameter of the fastener, which was then inserted in a fastener support fork. These two components were then mounted in a steel holder for stability (14). The fastener that would be tested rested on the fork. Then a compressive force was applied directly to the top of the blade to shear the fastener. Once the load drop reached 2%, the test was stopped, and shear strength was calculated.

Statistical modeling

Statistical analysis and modeling were conducted using JMP version 16. For mathematical modeling, neural networks via JMP were used to develop the model. All the available data was divided into three groups with 50% used for the training set, 25% used for the validation set, and 25% used for the test set. A detailed configuration of layers and units was shown in our neural network with five neurons within the hidden layer (**Figure 4**). Hidden units 1 through 5 (H1–H5) in the first hidden layer were adopted through a trial-and-error procedure to find the optimal number of neurons in the layer. The non-linear hyperbolic tangent activation function was used in the hidden layer. This system allowed the network to adjust all the adjustable coefficients/parameter by learning how to adjust them in a way that made the prediction the most accurate. This would maximize the coefficient of determination, which is the R2 value that provides information about the goodness of fit of a model.

In addition, Tukey's method via Minitab was used in ANOVA to create confidence intervals for all pairwise

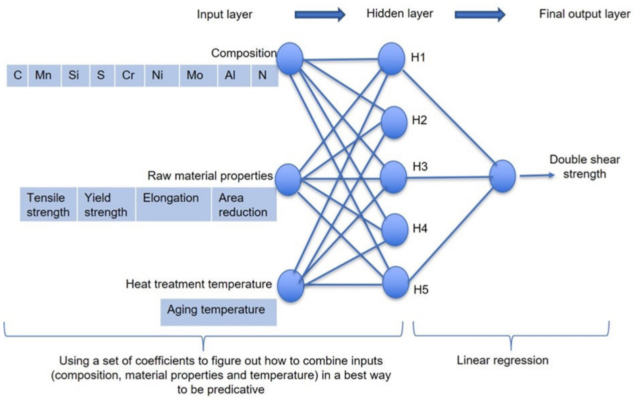

Figure 4. Neural network used in this evaluation. A standard feed-forward network with one hidden layer was employed to develop the model. The optimal number of units in the hidden layer was determined to be 5 (H1–H5) by a trial-and-error procedure where we examined from 1 to 8 units. The hidden layer (H1–H5) is located between the input and output. It performs nonlinear transformations of the inputs entered into the network.

differences between simulated and experimental strength data (8). Tukey's 95% confidence interval was calculated to determine the statistical significance of mean values for both simulated and experimental strength data.

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