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Prediction of Material Strength Properties by Materials Informatics

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In the past, strength properties of structural materials have been evaluated by destructive testing, however it was difficult to obtain and evaluate exhaustive data when the number of destructive tests increased, which was costly and time-consuming. Mitsubishi Heavy Industries, Ltd. (MHI) has established a technology to promptly predict material strength properties by applying informatic science, known as materials informatics, to structural metal materials. This technology is expected to contribute to the reduction of material strength variation, improvement of manufacturing yield, and advancement of life evaluation technology. This report describes case studies of applying the established technology to long steam turbine blades and high-temperature steam piping of thermal power plant.

1. Introduction

The strength properties of structural metal materials used in our high-temperature equipment are complicated with many influencing factors such as chemical compositions and heat treatment conditions, and quantitative evaluation of these properties by destructive testing is very costly and time-consuming. Recently, materials informatics (MI), which utilizes informatic science such as machine learning for material design, has been attracting attention, and examples of new material development in a short period of time by utilizing MI have been reported, mainly in the field of functional materials[(1)]. MHI has been applying MI to structural metal materials to rapidly predict the strength properties of materials in order to optimize manufacturing conditions and develop technologies for evaluating the life of products. This report presents an overview of our initiatives.

2. Optimal heat treatment condition prediction technology

Figure 1 shows the appearance of a long steam turbine blade we manufacture[(2)]. In manufacturing the long blade, procured round bar-shaped 17-4PH steel is forged into blade shapes, heat treated such as solution, stabilizing and aging, and then test specimens are taken from the excess portion of the long blade to check the tensile properties. In this tensile test, there are cases in which the 0.2% proof stress varies and does not meet our control range, resulting in repeated heat treatment or even disposal of the blade. The variation in 0.2% proof stress was assumed to be due in part to the variation in the chemical compositions of the material. Therefore, we considered the application of MI to predict the optimum aging heat treatment temperature (time is constant) which affects the strength, taking into account the chemical compositions, to reduce the variation of 0.2% proof stress in the tensile test. **Figure 2** shows the manufacturing flow of long steam turbine blades and an illustration of MI application.

Table 1 summarizes the conditions under which the prediction model was created through machine learning. For the learning and measurement of prediction accuracy, approximately 8,300 standardized data on the chemical compositions of materials, heat treatment conditions, and 0.2% proof stress obtained from tensile tests of long steam turbine blades we manufactured in the past

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were used (for preprocessing each piece of data, the deviation from the mean of all data was divided by the standard deviation of all data). Approximately 800 data, which corresponds to 10% of the total amount of data, were used as test data for measuring prediction accuracy, and the remaining approximately 7,500 data were used as learning data. Since there is the possibility of overestimating the prediction accuracy for unknown material charges if data of the same material charge are mixed in the learning and test data, the test data were extracted with consideration to avoid mixing data of the same material charge in the learning and test data. For explanatory variables, in addition to chemical compositions and heat treatment conditions, textual information that may affect the 0.2% proof stress, such as the type of heat treatment furnace used and the type of die used during forging, was also considered, and those contributing to improved prediction accuracy were selected.

Figure 1 Appearance of long steam turbine blade

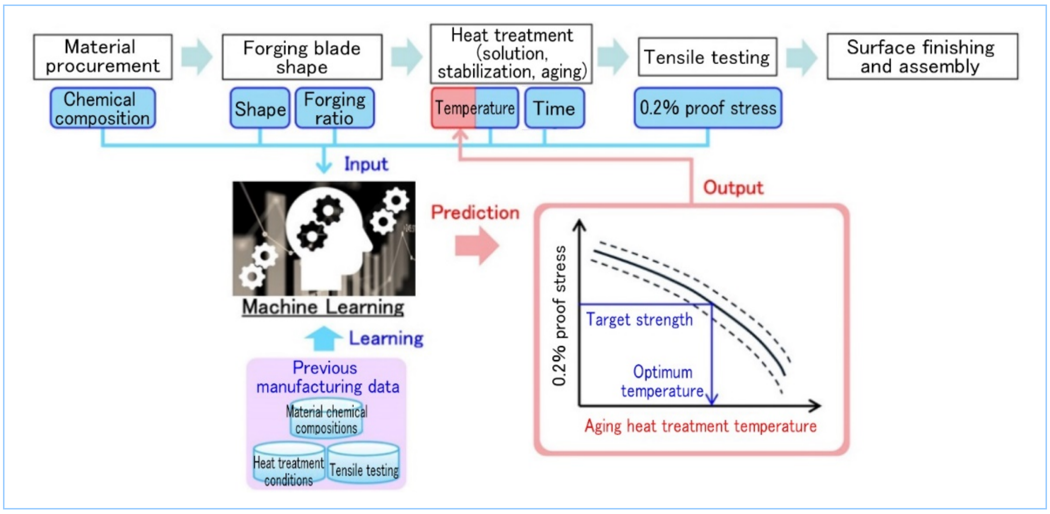

Figure 2 Long steam turbine blade manufacturing flow and MI application

Table 1 Summary of machine learning prediction model

Explanatory variable	- Chemical compositions (C, Si, Mn, P, S, Ni, Cr, Cu, Al, Nb+Ta, N, Ti) - Aging heat treatment temperature - Solution, stabilization, aging heat treatment time * Focused on aging heat treatment with respect to heat treatment temperature
Objective variable	0.2% proof stress
Algorithm	XGBoost
Number of learning data	Approx. 7500
Number of test data	Approx. 800

Four machine learning algorithms, Support Vector Regression(3), RandomForest(3), CatBoost(4), and XGBoost (eXtreme Gradient Boosting)(5), were used to create prediction models, and the prediction accuracy was measured on test data. We adopted XGBoost, the prediction accuracy of which was the highest. XGBoost is a method combining a technique called boosting and decision trees. Boosting improves prediction accuracy by creating multiple weak learners and repeating the operation where the next learner corrects the errors of the previous learner. We cross-validated XGBoost hyperparameters (number of decision trees, depth of decision trees, learning rate, etc.) among the learning data, and adopted the combination that resulted in the highest prediction accuracy.

Figure 3 compares the observed values (tensile test results) and machine learning predictions for the learning and test data. For both the learning and test data, the trends of observed and predicted values are generally consistent, indicating that the 0.2% proof stress trend can be predicted based on the chemical compositions and heat treatment conditions. Prediction accuracy was evaluated using the standard error shown in the equation(1).

$$SE = \sqrt{1/(n-p-1)\sum_{i=1}^{n}(y_i - f_i)^2} \qquad \cdots\cdots\cdots\cdots(1)$$

where SE is the standard error, n is the number of data, p is the number of explanatory variables, y_i is the observed value, and f_i is the estimated value. The prediction accuracy of the test data was $\pm 3SE = \pm 37.2$ MPa, which is smaller than our control range. However, due to the influence of using an algorithm with a decision tree, a continuous prediction of the relationship between aging heat treatment temperature and 0.2% proof stress is discontinuous and stepwise, as shown in **Figure 4**. This material has increased proof strength due to the Cu-rich phase that precipitates during aging heat treatment[(6)]. Considering that precipitation is continuously proportional to the temperature and time of aging heat treatment, it was assumed that the machine learning prediction results were inconsistent with the precipitation behavior of the Cu-rich phase and deviated from the actual substance, and it was considered that if the optimal aging heat treatment temperature was predicted by inverse problem analysis, the prediction accuracy may deviate from that measured by the test data. Therefore, as shown in the curve in Figure 4, the relationship between aging heat treatment temperature and 0.2% proof stress was obtained by predicting 0.2% proof stress through machine learning at a representative aging heat treatment temperature with a relatively large number of data and assumed high prediction accuracy, and then approximating the result by a quadratic polynomial approximation. The prediction accuracy of the test data was measured again using this method. The result was $\pm 3SE = \pm 37.8$ MPa, which is almost the same prediction accuracy as before the quadratic polynomial approximation was performed, and now the relationship between aging heat treatment temperature and 0.2% proof stress can be continuously predicted. **Figure 5** shows the probability density of 0.2% proof stress before and after MI application. By using MI to predict the optimum aging heat treatment temperature according to the chemical compositions of the procured material and applying it to the actual product, the 0.2% proof stress is expected to meet our control range at a higher probability than before.

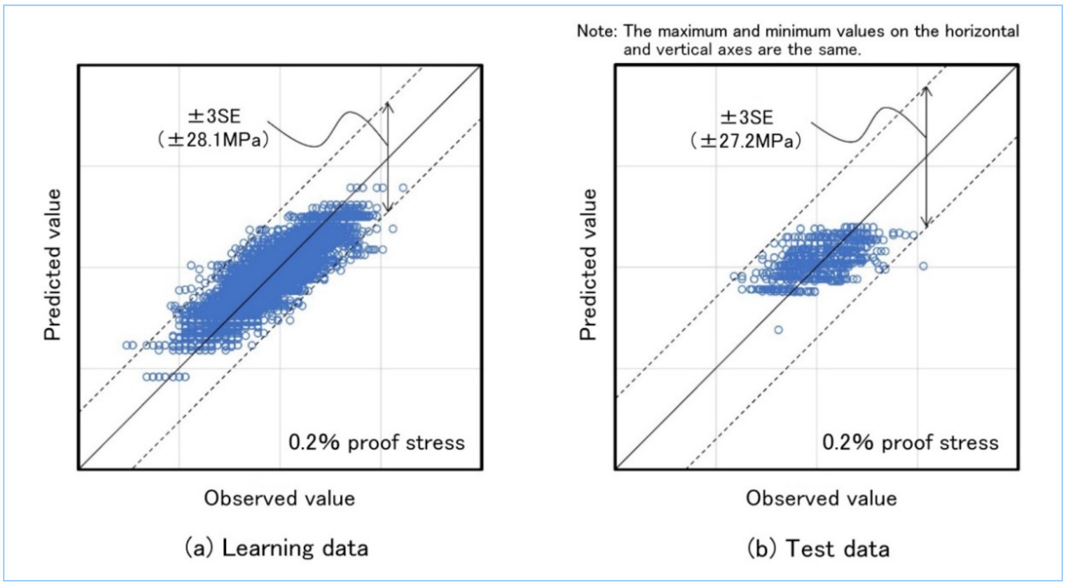

Figure 3 Comparison of 0.2% proof stress between observed values and machine learning predictions

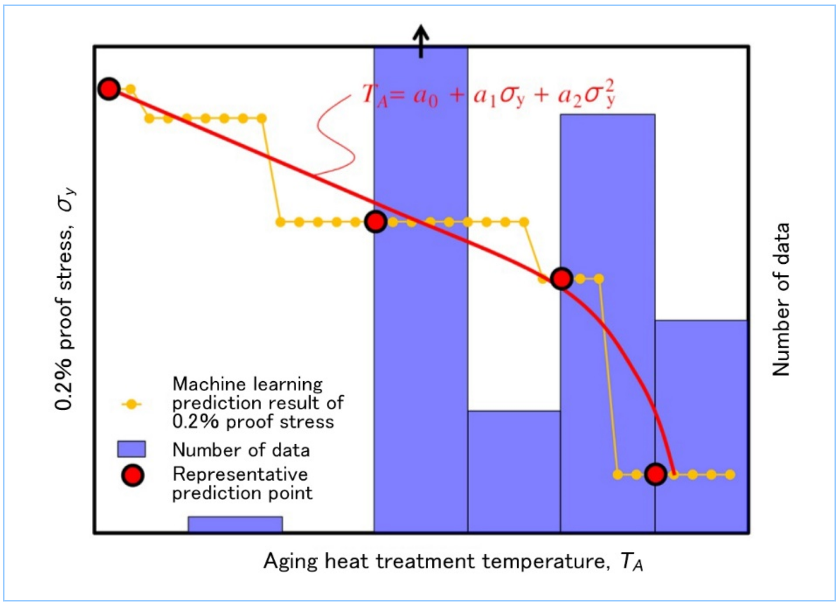

Figure 4 Relationship between aging heat treatment temperature, 0.2% proof stress and number of data

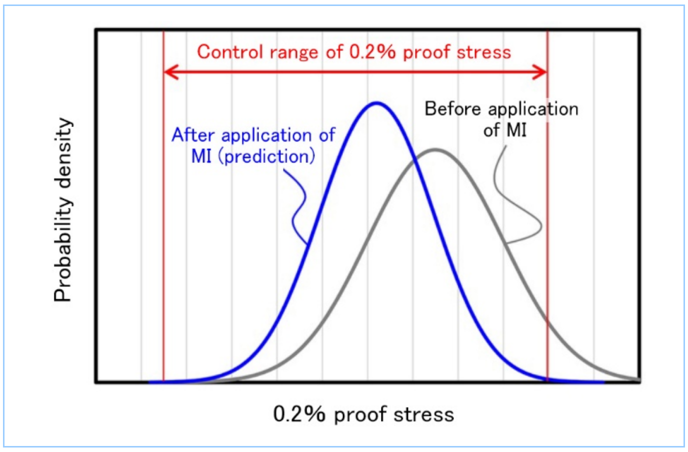

Figure 5 Probability density of 0.2% proof stress before and after MI application

3. Creep property prediction technology

Thermal power plants often use ferritic heat-resistant steels such as 9Cr-1Mo-Nb-V steel (The Interpretation for the Technical Standard for Thermal Power Plant KA-STPA28, ASME SA-335 P91) and 9Cr-1.8W steel (The Interpretation for the Technical Standard for Thermal Power Plant KA-STPA29, ASME SA-335 P92) as materials for high-temperature steam piping. For these materials, creep rupture data were collected for each steel grade, and creep life evaluation formulas were calculated using the LMP (Larson-Miller Parameter) method(7)(8) to predict creep life based on operating temperature and stress. However, since the data used to create the creep life evaluation equation are analyzed together, differences in creep rupture strength between material charges are not taken into account, and a certain amount of variation cannot be avoided in the predicted strength values. Therefore, even if a material charge has excellent creep rupture strength, materials with remaining creep life may be inspected early based on the life evaluation equation.

If we can evaluate creep life considering the variation among material charges and reduce the variation in creep rupture strength of materials to be procured, efficient maintenance management of thermal power plants will be possible, which contributes to preventing unplanned plant shutdowns and improving reliability. Therefore, we studied creep life prediction technology that factors in chemical compositions and heat treatment conditions by MI, conducted sensitivity analysis of chemical compositions that affect creep rupture strength, and examined material specifications that can reduce the variation of creep rupture strength. This report describes a case study of 9Cr-1.8W steel.

Table 2 summarizes the conditions for creating a creep life prediction model through machine learning. For learning and measurement of prediction accuracy, creep rupture data of base metal and welded joints of ferritic heat-resistant steel we acquired, and creep rupture data of base metal of ferritic heat-resistant steel from the NIMS Creep Data Sheet(9), about 1,680 data in total were standardized and used. For measurement of prediction accuracy, about 100 data of 9Cr-1.8W steel with a rupture time of more than 1,000 hours were extracted and used, and the remaining approximately 1,580 data were used as learning data. Also in this case, the test data were extracted considering the material charge so that data of the same material charge would not be mixed in the learning and test data, and the prediction accuracy was verified for unknown material charges. The machine learning algorithm used was CatBoost, which had the highest prediction accuracy. Like XGBoost, the CatBoost is a method that combines boosting and decision trees, and is characterized by its superior handling of textual information. Other methods for creating the prediction model are the same as those described in Chapter 2.

Table 2 Summary of machine learning prediction model

Explanatory variable	- Chemical compositions (C, Si, Mn, P, S, Ni, Cr, Mo, V, Nb, Al, N, W, B, Cu, Ti, N/Al) - Normalizing, tempering, and post-weld heat treatment temperature and time - Material shape (tube, pipe or plate) - Material thickness - Base metal or welded joint - Creep test temperature and stress (normal logarithm)
Objective variable	Creep rupture time (normal logarithm)
Algorithm	CatBoost
Number of learning data	Approx. 1580
Number of test data	Approx. 100

Figure 6 compares the observed values of the test data (the ordinary logarithm of the rupture time in the creep test) with the predicted values through machine learning. The observed and predicted trends of the test data were generally consistent, indicating that the creep life trend can be predicted considering the chemical compositions and heat treatment conditions. This technology enables creep life evaluation that factors in variations in material chemical compositions, even for the same steel grade, and we use this technology in combination with the conventional LMP method for screening of inspection points, etc.

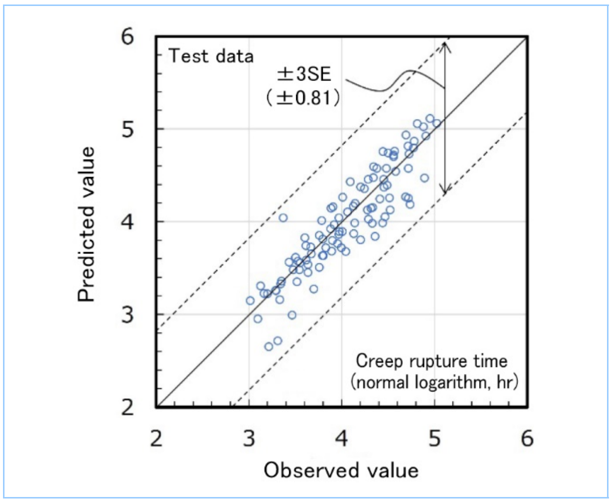

Figure 6 Comparison of creep rupture time between observed values and machine learning prediction results

Figure 7 shows the partial dependence plots of Mo, N, W and N/Al (ratio of N to Al) for 9Cr-1.8W steel. Partial dependence plots are machine-learning predictions of the average behavior of the objective variable when an explanatory variable is changed. In this case, only creep rupture data over 60,000 hours for 9Cr-1.8W steel were used to create partial dependence plots to check the effect on creep rupture strength, especially over the long term. Mo was assumed to have a small effect on the creep rupture time when varied within the range of the standard (ASME SA-335 P92). On the other hand, N, W, and N/Al were found to have an effect on the creep rupture time. N showed a tendency to increase the creep rupture time with increasing additions up to about 0.05%. This is assumed to be because the 9Cr-1.8W steel was precipitation strengthened by MX ((Nb, V) (N, C))(10), which contributed to an increase in the amount of MX nucleation up to about 0.05%. It was found that W had a tendency of increasing the creep rupture time when the content was greater than about 1.7%. This is assumed to be because W contributed to the increase in creep rupture strength as a solid solution strengthening element in this grade(11). N/Al showed a tendency that with its increase up to about 4, the creep rupture time increased. This is assumed to be because a larger N/Al resulted in a larger amount of effective N that did not bond with Al but became MX and contributed to precipitation strengthening(12). In the past, it was difficult to quantitatively evaluate the optimal chemical composition ranges due to high experimental costs and long testing times required. However, by applying MI, quantitative evaluation can now be performed. By incorporating the results of these MI evaluations into material purchase specifications as appropriate, we are studying to reduce creep rupture strength variation and prevent the purchase of low-strength materials.

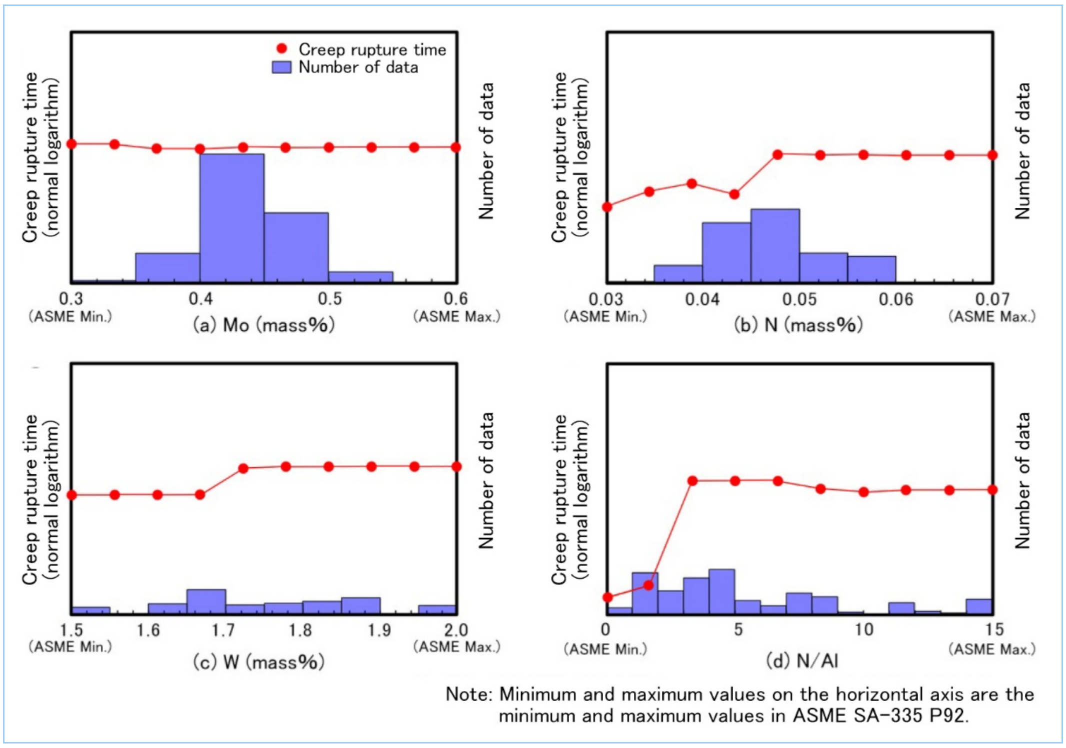

Figure 7 Partial dependent plot for creep rupture time for 9Cr-1.8W steel

4. Conclusion

By applying MI to structural metal materials, it is now possible to predict material strength properties of metal materials based on previously acquired data. In the case of long steam turbine blades, by creating a machine learning prediction model for 0.2% proof stress, we are able to predict the optimum aging heat treatment temperature according to the chemical compositions of the procured material and it was found that by applying it to actual products, the 0.2% proof stress is expected to satisfy our control value with a higher probability than before. For ferritic heat-resistant steel used for high-temperature steam piping in thermal power plants, it is now possible to predict creep life in consideration of chemical compositions and heat treatment conditions. In addition, by utilizing MI, we are able to perform quantitative sensitivity analysis of chemical compositions that affect creep rupture strength and it was found that the variation in creep rupture strength could be reduced and the purchase of low-strength materials could be prevented.

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