Research article

Enhanced processing map of Ti–6Al–2Sn–2Zr–2Mo–2Cr–0.15Si aided by extreme gradient boosting

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1. Introduction

(a + β) Ti alloys have been widely used in various industries due to the superior specific strength, corrosive resistance, and biocompatibility [1, 2]. Ti–6Al–2Sn–2Zr–2Mo–2Cr alloy was developed in 1970s to improve mechanical properties, particularly strength and wear resistance, as compared with Ti–6Al–4V [3]. Si was added to this alloy later, denoted as Ti–62222S, to further enhance mechanical properties [4]. Nevertheless, a high-temperature thermomechanical process of Ti–62222S often causes undesirable microstructural evolutions, thereby degrading a material formability [5]. To avoid such a problem, researchers have introduced a processing map to anticipate “safe” processing conditions (i.e., deformation temperature and strain rate) [6]. Processing map requires a huge amount of data to establish, resulting in the necessity for vast experimental resources. There have been many efforts to reduce the number of experiments by various predictions and modeling, such as a constitutive approach [7]. However, this method is often inappropriate for prediction as it requires establishing a physics-based model to fit the obtained data [8].

The recent rise of machine learning is attributed to its capability of solving nonlinear multi-variable problems. High-temperature deformation behavior of Ti alloy is nonlinearly affected by various factors, which can be effectively solved through machine learning. Indeed, there have been several endeavors to predict a high-temperature flow curve [9, 10, 11, 12] or to plot a processing map [13, 14, 15] of Ti alloys using machine learning. However, most of these studies employed the artificial neural network (ANN) as a machine-learning approach; they either compared ANN with a constitutive approach [10, 11] or tried to improve ANN performance [13]. Few exceptional studies [12, 15] adopted the genetic algorithm and support vector regression for their prediction. It is still required to verify other machine-learning algorithms, particularly the variants of gradient boosting.

The authors recently suggested the advantages of extreme gradient boosting (XGB) for metallurgy; in the given problem, XGB was superior to ANN in both aspects of predictability and efficiency [16]. Therefore, this study employed XGB to plot an enhanced processing map for the first time. The term “enhanced” here indicates an increasing predictability for a formability with the less number of experiments.

2. Material and methods

The chemical composition of the investigated Ti–62222S was Ti–5.90Al–2.01Sn–1.97Zr–1.98Mo–2.03Cr–0.22Si–0.002N–0.130O in mass percentages. The ingot was hot-forged at 1403 K, quenched in a water bath, forged again at 1183 K, and then cooled in an ambient atmosphere. The microstructure of the forged billet was investigated using...
electron backscatter diffraction (EBSD) analysis. The sample was water-abraded using #400 emery paper and then electropolished at 253 K in a solution of 50% CH₃OH, 30% C₄H₉OH, and 20% HClO₄.

To obtain the mechanical data for machine learning, the billet was machined into cylindrical specimens with 10 mm in diameter and 15 mm in height. Connected to thermocouples, they were compressed to 4.5 mm using Gleeble 3800 GTC machine at the target temperatures of 1073, 1173, and 1273 K, respectively. The employed strain rates were 10⁻³, 10⁻², 1, and 10 s⁻¹, respectively. Such deformation conditions were established based on the literature plotting a processing map of Ti–6Al–4V alloy [17, 18, 19, 20, 21, 22, 23]. The highest strain rate was controlled by the stroke mode of Gleeble software, while the others were performed in the strain mode. Ta foil was placed between the press and specimen to inhibit adhesion. Graphite lubricant was applied to both surfaces of specimen to mitigate shear localization by friction [24].

3. Machine learning and processing map

The compressive tests provided 24,875 examples with four features of temperature, strain rate, strain, and stress. 6543 examples in the strain range of 0.1–1 were chosen for the machine learning of the steady-state region that had a crucial effect on plotting a processing map. Data for each feature were standardized using the average and standard deviation. The flow curves obtained at a strain rate of 10 s⁻¹ were designated as the testing dataset, because they are the most difficult to predict due to the extreme environment and extrapolating condition. The remaining examples were randomly divided into the training and validating data-sets, respectively, at the ratio of 8:2. The hyperparameters were optimized through the grid search algorithm.

4. Results and discussion

Figure 1 shows the initial microstructure of the investigated Ti–6222S. The micrograph indicated the typical bimodal structure composed of equiaxed α grains and lamellar (α + β) colonies. This microstructure is understood by the employed forging temperature (1183 K) lower than the β-transus temperature of Ti–6222S (1238 K [4]). The average diameter of primary α grains was measured to be 10.4 μm, which was consistent with the literature [25]. The area fraction of α phases (93%) was higher than the literature data [25] due to the omitted fraction of narrow β lamellae in Figure 1.

Figure 2 presents the entire flow curves obtained from the compressive tests. The elastic regime ended before strain of 0.1 for all cases, which was excluded from the machine learning. Flow stresses decreased with increasing deformation temperature and decreasing strain rate. The flow curves generally reached the maximum strength at the early stage of plastic deformation, followed by steady state or gradual decrease of stress. It should be noted that the flow curves obtained at 10 s⁻¹ exhibited the different tendency; the curve deformed at 1073 K showed the flow...
softening (Figure 2a), whereas those at the higher temperatures presented the flow hardening (Figure 2b and 2c). The same tendency was confirmed in Fe–10Cr–0.15C subjected to Gleeble compressive test [26].

Figure 3 compared the predicted flow curves at 10 s⁻¹ with the experimental results. Such a strain rate is the extrapolating condition, and thus the most difficult to predict. The XGB model provided a good prediction at 1173 and 1273 K. However, the predicted data deviated from those at 1073 K. The data used for the machine learning were biased towards the flow hardening at 10 s⁻¹ as there was the only case (i.e., 1073 K) exhibiting the flow softening at such a high strain rate. This bias is further discussed below.

Figure 4 compared the three processing maps. Excluding the data of 10 s⁻¹ resulted in the incomplete processing map (Figure 4b), which was totally different from the complete one (Figure 4a). The XGB prediction for the omitted data recovered the accuracy (Figure 4c), particularly in the instability map, as marked with the gray areas. Figure 4a and 4c exhibited the consistent range of instability conditions (i.e., <1140 K and >10⁻¹.7 s⁻¹) in contrast to those in Figure 4b (<1100 K and >10⁻¹ s⁻¹).

The predictability for the power dissipation map significantly varied with a strain rate. The XGB model precisely estimated the high-η range (>0.3550) at low strain rates, as marked by the yellow areas in Figure 4a and 4c. This is a remarkable enhancement as compared with the range shown in Figure 4b. On the other hand, both contours of Figure 4b and 4c deviated from those of Figure 4a at high strain rates (>10⁻¹ s⁻¹). The poor prediction of machine learning in this regime arose from the biased data towards the flow hardening at 1 s⁻¹, as mentioned above. Alleviating such a bias can further improve the machine-learning predictability. In specific, it is recommended to employ the binary feature to define the type of flow curve (i.e., flow softening or hardening).

Another strategy for enhanced predictability is to consider the effect of adiabatic deformation heating. Semiatin et al. [27] attributed the flow softening of Ti–6Al–4V to two factors: (i) deformation heating caused by a low thermal conductivity and (ii) bending and kinking of lamellar microstructure. The latter factor had a smaller contribution to the present alloy, because it had the bimodal microstructure (Figure 1) in contrast to the full lamellar structure of the reference material [27]. Meanwhile, Xiao et al. [28] ascribed the flow hardening at 10 s⁻¹ to change from dynamic recrystallization to dynamic recovery with increasing strain rate. The phenomenon results from an increased β fraction induced by the deformation heating. Consequently, the integration of deformation heating is expected to enhance the predictability of machine-learning model for a processing map.

The deformation heating can be integrated with the machine-learning model in two ways. The nominal compressive test may be alternated with a load-unload-reload test [29] that minimizes the deformation heating. However, this method does not provide a continuous flow curve anymore, and thus may decrease the machine-learning predictability. Instead, a constitutive equation can be considered to obtain a continuous flow curve compensating the effect of adiabatic deformation heating [30]. This approach has an additional benefit to minimize the effect of friction, of which the extent increases with increasing strain rate [31].

Finally, it is worthwhile noting the reduced computing resource by using XGB algorithm. The XGB-based model spent 0.5 h for learning the data and yielding the expectation for the present case, which was significantly faster than ANN taking 2.3 h. Such a rapid learning is the inherent advantage of XGB algorithm. Yu et al. [16] compared the same algorithms in predicting a nonlinear temperature change of Mg alloy caused by an electropulse. The authors reported the 1000-fold faster learning of XGB compared with ANN, as consistent with the present results. It is considered that the variants of gradient boosting have a higher learning speed than that of multilayer perceptron approaches. In conclusion, XGB has a high potential for enhancing a processing map of Ti alloys.

5. Conclusions

This study employed XGB for the first time to enhance a processing map of Ti–62222S with a less amount of experiments. The predictability of XGB was improved by the proper selection of learning examples and the optimization of hyperparameters. Compared with the incomplete processing map, the XGB-aided map was enhanced with the higher accuracy in the instability map and the low-strain-rate power dissipation map. The deviation at high strain rates resulted from the bias, which would be improved by employing the binary feature and integrating the effect of adiabatic deformation heating. This study has proven the potential usefulness of XGB for enhancing a processing map.

Declarations

Author contribution statement
Min Hwa Bae: Performed the experiments; Analyzed and interpreted the data; Wrote the paper.
Minceob Kim: Performed the experiments.
Jinyeong Yu: Conceived and designed the experiments; Performed the experiments.
Min Sik Lee: Analyzed and interpreted the data.
Sang Won Lee: Conceived and designed the experiments; Contributed reagents, materials, analysis tools or data.
Taekyung Lee: Conceived and designed the experiments; Contributed reagents, materials, analysis tools or data; Wrote the paper.
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Data availability statement

Data will be made available on request.

Declaration of interests statement

The authors declare no conflict of interest.

Additional information

No additional information is available for this paper.

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