Design of Dual-Phase Steel Based on Active Learning

Jincheng Wang[1]*, Xiaobing Hu[2], Junjie Li[1]
1. State Key Laboratory of Solidification Processing, Northwestern Polytechnical University, Xi'an 710072, China
2. Xi'an Rare Metal Materials Institute Co. Ltd, Xi'an 710016, China
*Corresponding address: e-mail: jchwang@nwpu.edu.cn

Abstract: Dual-phase (DP) steels are an important family of steel grades widely used in the automotive industry, aerospace, ultra-supercritical generating units, etc.Reducing costs throughout the process from raw material preparation to experimental design is a critical challenge that needs to be addressed urgently. This paper develops an effective active machine learning (AL) method to explore and exploit new DP steels with excellent mechanical properties. A simple case of hardness optimization is first reported to validate the reliabilityand efficiency of the AL method. Simultaneous enhancement of strength and plasticityis then realized by fast learning in a vast design space free of Co, finding several desired low-cost DP steels. More importantly, convenient application software has beensuccessfully developed, which has practical significance for the engineering application of the AL method.

Keywords: Dual-phase steels； active learning, mechanical properties.

1 Introduction

DP steels have potentialmechanical properties, making them widely applied in the automotive industry, aerospace, ultra-supercritical generating units, etc. Uncovering the complicated interaction between compositions/processing, microstructures, mechanical properties is extravagant in terms of time andmoney by traditional trial-and-error. Therefore, it is necessary to develop a new method to accelerate the design of DP steels.

A potential solution to the problem above is machine learning (ML),which can quickly explore the complex composition space to improve the microstructure and mechanical properties. However, the prediction was only induciblefor the samples near the training data. To solvethis problem, an adaptive active learning (AL)method is a wise direction for the iterative experiments.To the design of DP steels, one is bound to meet a sparse and small dataset. The efforts should beperformed in early iterative experiments before adaptive sampling to balance data distribution as much as possible (reducethe overall σ of ML prediction), which may be beneficial for the subsequent search for the global optimum.

In this study, an improved AL method is proposed, and validated for its ability in finding global optimum by only several iterations, then used to design new strength-plasticityenhanced DP steels free of Co.

2 Experimental procedure and AL method

Experimental procedure

The DP steelswere prepared using a mold of a WKII model vacuum arc melting furnace. Homogenization, hot-rolling, and heat treatment were executed sequentially to ensure appropriate microstructure.

3 AL method

We trained a Gaussian process regression (GPR) model. Employing the model, we then ranked the samples by their σ of prediction. Three top-ordered candidates were recommended to experiment and then feedback to the initial set, which ensures a rapid reduction of σ on the design space.This procedure was repeated several times until GPR generated a stable prediction for the unexplored alloys. Subsequently, EI was used to explore the region wherethe alloys have a superior property than the best-so-far until anoptimal candidate was found.To enhance the strength and plasticitysimultaneously, some expert experience is brought in ML.

4 Result and discussion

Validation of the AL method in finding global optimum

Executing the AL method, we explored a total of 27alloys in the designspace. As shown in Fig.1a, we first extracted the candidates with large σ in the 1–6iterations, their hardness varies over a widerange (≈10–55 HRC). Fig.1b reveals that the predicted σ ofthe ensembles in the virtual set rapidly decreases and convergesto the position where the mean is ≈5 during the 1–4iterations. Interestingly, the curves seem to change slightly in the 4–6iterationsand a stable plateau of σ occurs, demonstrating negligible benefits from the sequentially recommended alloys according to exploration.At the first exploration stage, the variation of average EI with iteration is ruleless, as shown in Fig. 1(c). When the extremely sparse region in the design space is filled, the new recommended alloys tend to minimize σ, and EI is therefore reduced, just as displayed in the 4-6 iterations in Fig. 1(c). Once the improvement of data distribution is completed, exploitation starts, the reduction of EI decreases, and the new alloy approaches the global optimal, as depicted after the sixth iteration in Fig. 1(c). Notsurprisingly, the mean absolute error (MAE) between the predictions and the measurements quickly drops in iterations 1–4, asshown in Fig.1(d) but fluctuates slowly in iterations 4–6, revealing that the alloys recommended by ranking σ haveinsignificant contribution to the improvement of the predictionprecision on the design space after the fourth iteration, as shown in Fig. 1(f). MAEs in the last three iterations are thus close to 0.

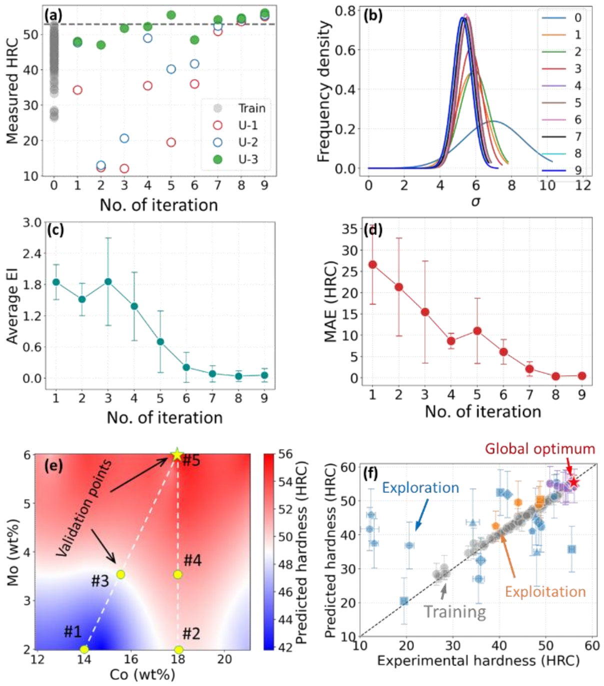

Fig.1 Design process of DP steels with the highest HRC. (a) Experimental HRC *vs* iterations. (b) Frequency density of σ in 9 iterations. (c) EI *vs* iterations. (d) MAE *vs* iterations.(e) Predicted HRC of Fe-0.05C-12Cr-1Ni-Co-Mo DP steels.(f) Experimental validation of the designed alloys.

5 Application of the AL method to design strength-plasticity enhanced DP steels free of Co

The experimental dataset with the variates of Ti, Mo and W was constructed, and GPR model was used to learn the relationship between chemical compositions and the properties (UTS and elongation at 650 ℃), as shown in Fig. 2(a)-(f). Our designed steels show the highest product as shown in Fig. 2(h), followed by the 15Cr steelsmarked by the gray arrow. In addition, the product of steel D3 is156%, 31%, and 62% higher than the best ones in 9Cr, 15Cr, and20Cr steels, respectively. The product of V1 shows an increase ofapproximately 33% compared to that of the steel marked by thecyan arrow. Moreover, our designed steelsare free of Co and contain low Ni content (5 wt%–8 wt%), and the exploitation cost is thus lower thanthat of traditional DP steels.

6 Conclusion

The design, validation and application of the AL method are successfully realized by finding new DP steels free of Co. The main conclusions are summarized as follows:

1. An accurate and high-efficiency AL method is developed, which achieves both data distribution optimization and high-property alloy exploitation.
2. The DP steel with the highest hardness was successfully designed from a given composition space,

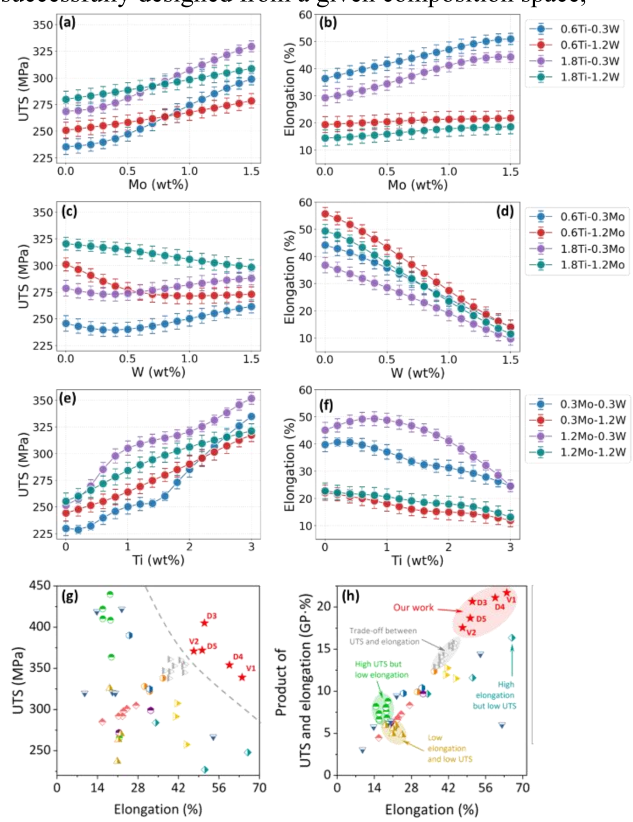

Fig.2 Design process of DP steels free of Co with enhanced strength and plasticity. (a)-(f) Predicted effect of Ti, Mo and W contents on UTS and elongation. (g) UTS vs elongation and (h) Product of UTS and elongation vs elongation for the typical 9-12Cr, 14Cr, 15Cr and our designed steels.

which uncovers the capability of global optimization of the AL method.

3. Several new low-cost 15Cr DP steels are designed.

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References

[1] Q. Wu, Z. Wang, X. Hu, et al., Uncovering the eutectics design by machine learning in the Al–Co–Cr–Fe–Ni high entropy system, Acta Materialia 182 (2020) 278-286.
[2] X. Hu, J. Wang, Y. Wang, et al., Two-way design of alloys for advanced ultra supercritical plants based on machine learning, Computational Materials Science 155 (2018)331-339.
[3] C. Guo, X. Hu, X. Han, et al., Laser Precise Synthesis of Oxidation-Free High-Entropy Alloy Nanoparticle Libraries, Journal of the American Chemical Society 146 (2024) 18407-18417.