Active learning-enabled the discovery of ultra-high saturation magnetization soft magnetic alloys

Yahao Li[a], **Yicong Ye**[a]

[a] *Department of Materials Science and Engineering, National University of Defense Technology, Changsha, China 410073* liyahao16@nudt.edu.com

1. Introduction

Alloy design has long been a knowledge-guided approach coupled with experimental trial and error. However, facing high-entropy alloys (HEAs) with complex compositions and large design space, traditional experimental methods often fail. In this paper, an active learning (AL) framework is proposed to achieve the discovery of ultra-high saturation magnetization strength (M_S) alloys based on limited data[1].

2. Results and discussion

In order to design an ultra-high M_S alloy, we devised a research strategy as shown in Fig.1. In this framework, we first perform active learning validation on the dataset, while comparing different ML models and acquisition functions to select the combination with the highest active learning efficiency[14]. The selected efficient AL engine is further used to perform an active learning loop to discover high M_S alloys through continuous iterations. During the AL validation part, we use 20% of the dataset to train the surrogate model in AL and 80% as the search space for model exploration. The purpose is to simulate that the real search space is much larger than the actual dataset available. In addition, to avoid the chance of data allocation, we randomly split the data 100 times to calculate the average value of AL efficiency.

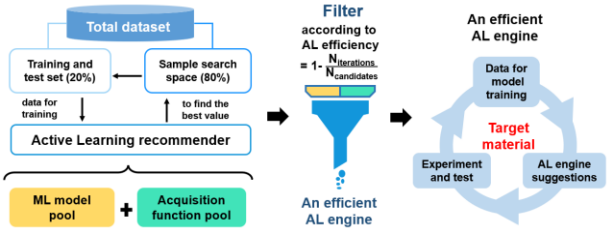

Fig. 1: Overview of the active learning strategy.

The combination of GPR+EI was further used to form an efficient AL engine to carry out high M_S alloy design. For $Fe_xCo_yNi_zAl_uSi_v$, the elemental mass fraction intervals are set to $20 \le x \le 100$, $0 \le y \le 50$, $0 \le z \le 35$, $0 \le u \le 10$, $0 \le v \le 10$, and the step size is set to 1. The final composition space contains 110,198 alloys. When setting the range of elemental mass fraction intervals, the main reference is the upper and lower limits of the mass fraction of each element in the dataset, and the mass fraction interval of each element is adjusted by combining with the knowledge of the materials expert.

The M_S values of the 3 recommended alloys for each AL iteration are shown in Fig.4(a). The compositions and M_S of a total of 9 experimental alloys for the 3 iterations are given in Table S3. The hysteresis loops for each iteration of alloy testing are shown in Figure S2. Compared to the highest value of 218 emu/g for $Fe_{65}Co_{35}$[2] in the original data set, a new composition is greater than this value in each iteration: $Fe_{80}Co_{14}Ni_5Si_1$ (218.49 emu/g), $Fe_{70}Co_{25}Ni_4Si_1$ (225.76 emu/g) and $Fe_{66}Co_{28}Ni_3Al_1Si_2$ (219.33 emu/g), demonstrating the superior compositional design capability of AL. One of the formulations 2-3 as shown in Fig.2(a), $Fe_{70}Co_{25}Ni_4Si_1$ achieved an increase of 3.6% compared to the maximum value in the data set. We notice that the M_S of alloy 2-1 is actually unsatisfactory, which could be attributed to the component point lying within an unexplored interval, where the model predicts with a large uncertainty. The EI acquisition function includes both the predicted value and their uncertainty, leading to a large value of the calculated EI, which in turn results in the point being filtered out as a recommended point. Fig.2(b) shows the change in the RMSE of the model after each iteration with the recommended components added to the dataset. It reveals that the performance of the surrogate model continuously improves as the AL is performed. This is also reflected in the results of the third iteration in Fig.2(a). As the iteration increases, the model's prediction accuracy of the search space improves, the uncertainty decreases, and the experimental values of the performance of the model's recommended component points appear to be concentrated in the direction of the maximum. Therefore, the 3 recommended components are basically high-M_S alloy formulas in iteration 3, and there is no longer a situation similar to that of the No. 2-1 formula.

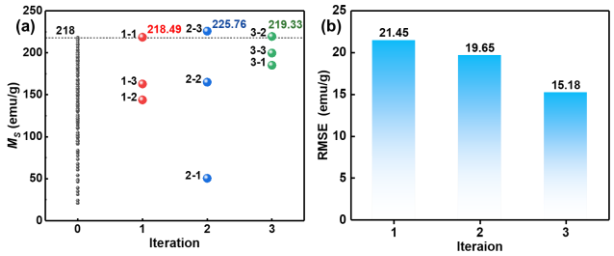

Fig. 2: (a) The results of 3 AL iterations, and (b) the prediction accuracy of the surrogate model after each round of AL.

It turns out that the effectiveness of our framework in rapidly designing soft-magnetic HEAs with elevated M_S.

References

[1] Y.H. Li and Y.C. Ye. Active learning-enabled the discovery of ultra-high saturation magnetization soft magnetic alloys. *Scripta Materialia*, 257, 116485, 2025.

[2] P. Saraswathi, and S. Madeswaran. Study on magnetic and structural properties of Fe65Co35 soft magnetic alloy prepared by arc melting and subsequent annealing. *Results in Materials*, 100509, 2024.