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Review paper

ARTIFICIAL INTELLIGENCE CHALLENGES IN MODERN ALLOYS DESIGN

Aleksandra Milosavljević[1a], Ana Kostov[1b], Marijana Pavlov-Kagadejev[1c]

[1] Mining and Metallurgy Institute Bor, Alberta Ajnštajna 1, 19210 Bor, Serbia
[1a] aleksandra.milosavljevic@irmbor.co.rs, 0000-0003-3841-7357
[1b] ana.kostov@irmbor.co.rs, 0000-0001-6436-9091
[1c] marijana.pavlov@irmbor.co.rs, 0000-0003-1090-6351

Abstract
Artificial intelligence (AI) is used in everyday research and in all fields, including materials science. Various AI models can predict the optimal chemical compositions, mechanical properties, microstructure and phase transformations of materials instead of long-term experiments or expensive simulations, especially for multicomponent alloys. However, its application, in addition to multiple advantages, also brings numerous challenges. This paper presents a brief overview of these challenges in modern alloy design.

***Keywords**: alloys, artificial intelligence, challenges, design*

1. INTRODUCTION

Materials science is very complex and demanding because of its essence - finding and developing new materials with certain properties, at the lowest possible cost and respecting environmental requirements. It is not at all an easy task, bearing in mind that it is necessary to conduct a lot of experiments under certain conditions. As the conditions for conducting experiments become more complex, the cost of experiments increases, as well as the duration. In order to save money and time, various forecasting methods, as well as simulations, have been developed. All these predictions and simulations were still limited, so over time the need for even more universal solutions grew.

With the progress of artificial intelligence, new possibilities have opened up. AI models use large data sets to be able to predict the properties of materials with high accuracy, and are therefore applied in all stages of the creation of a new material - from design to characterization, even in spectroscopy and electronic microscopy [1]. There are numerous examples of AI applications in alloys, and some of them have been experimentally confirmed [2,3,4,5].

As one of the few examples where machine learning (ML) models proposed the composition of a new alloy with improvements, it can be mentioned Ni-based superalloy [4]. In order to optimize physical properties (up to 11 parameters), the researchers used a artificial neural network (ANN). The network trained on existing experimental data. New Ni-base superalloy was designed and has the optimal properties (some of them better than previous) and cost [4]. Experimental tests confirmed that oxidation resistance and yield strength for this new alloy are superior to existing commercial superalloys [4].

This example clearly shows how AI can predict the optimal chemical composition and thus save us from expensive and time-consuming experiments. However, it is necessary to look at the other side, that is, the challenges that may arise when it comes to the alloys design.

2. CHALLENGES

One of the key problems is the lack of sufficiently large, high-quality and consistent dataset. Most of the existing data on alloys comes from different sources (literature, experiments, simulations). These data are often not standardized, and depending on the type of alloy, the available data may be limited, which makes it difficult for training AI models.

In multicomponent systems, there are a large number of combinations of elements that need to be processed and a large number of data that need to be collected. It represents an obstacle to finding the regularities based on which AI models will propose optimal solutions.

As an example, a machine learning approach for developing heat-resistant aluminum alloys with 15 alloying elements and 6 different heat treatment conditions was given in work [6]. The data set consists of aluminium alloys composition, heat treatment conditions and tensile test temperatures, while the ultimate tensile strength (UTS) values are output. In Figure 1a comparison of results with and without descriptors is shown. The presence of descriptors is better because the information about elements (physical, crystal, and chemical information) is more reliable then. Various models were compared based on the cross-validation (CV) results using the mean absolute error (MAE) as the scoring metric within the training set [6] and the values of R^2 for training and testing sets are given in Figure 1b.

It should be noted that this data set was for Al alloys obtained by conventional casting [6] which refers to another challenge – generalization of model and the lack of universality. Models trained on certain classes of alloys often cannot be easily applied to other systems.

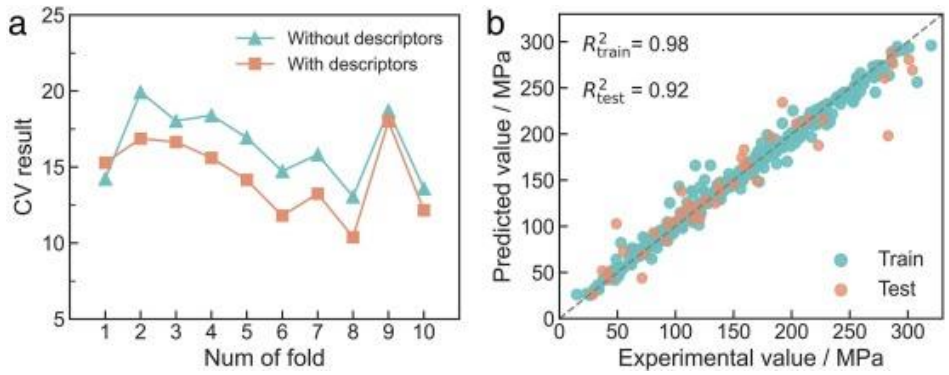

Figure 1. a Comparison of CV results with and without additional descriptors; b fitness based on the training set and testing set. [6] used under the terms of CC-BY-NC-ND

Considering that the microstructure of alloys depends on many factors (composition, cooling rate, heat treatment, deformation), it is very difficult to generate AI models that would predict the microstructure of a specific alloy. Therefore, the integration of artificial intelligence with thermodynamic models and simulations (CALPHAD) is desirable [7].

As an example, integration of various AI techniques along with thermodynamic calculations was used in design of refractory high entropy alloys (RHEA), which are very suitable for applications in extreme conditions [7]. In this study, metaheuristic methods, thermodynamic calculations and artificial neural networks (ANNs) were combined in order to specify and identify certain RHEA alloys [7]. The results were proved by experiments on $Ti_{17.5}Nb_{17.5}Zr_{13.5}Ta_{15.5}Mo_{17.5}V_{18.5}$ alloy [7]. Despite extensive testing, it can be said that even after this combination of models, certain limitations remained, but progress was made for the future directions.

So, the big problem in design of new alloys is the lack of data. In this scientific area, it is very important to know why certain composition or microstructure leads to certain properties, not just to get a prediction. Consequently, experimental confirmation is still necessary. An additional challenge related to the need of experiments is that there is a difference between experiments in laboratory conditions and the real environment in industry.

Considering the complexity of alloys, a multi-functional approach is needed with large dataset, both theoretical and experimental means, it is necessary to combine various types of knowledge. An integration of external knowledge, tools, logic, reasoning, etc. can be effectively implemented through the deployment of a multimodal multiagent AI system driven by large language models (LLMs) [8]. Multiagent systems produce new knowledge from various external resources from literature through databases to simulations. In Figure 2, the multimodal multiagent approach is shown as a multi-functional approach to materials design, which can ensure improvements in solving some of the challenges mentioned above.

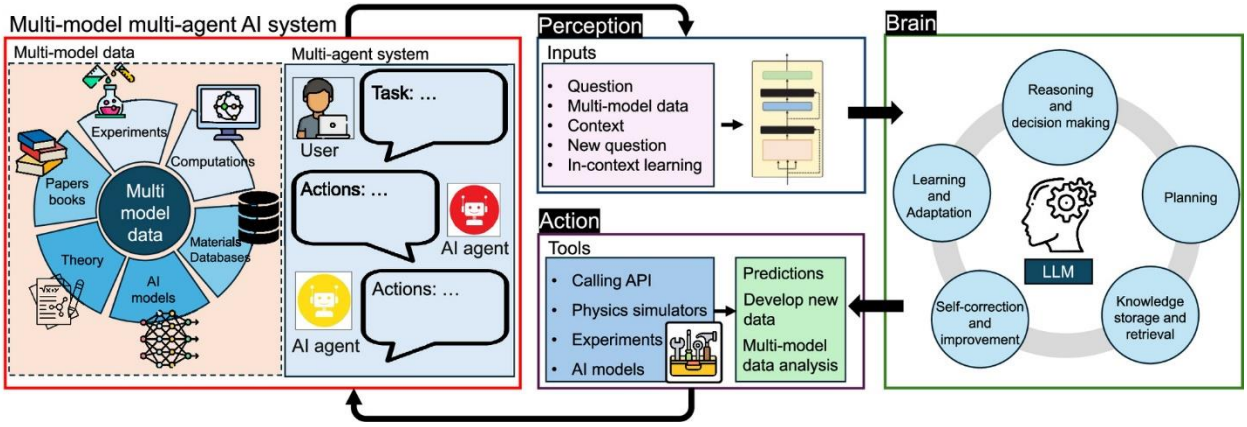

Figure 2. Multimodal multiagent approach as a flexible modeling strategy for materials discovery, modeling, and prediction. Multiagent modeling can extend the power of large-language models by enabling the integration of multimodal data from diverse sources, including simulations, experiments, materials databases,and theoretical models. [8] used under the terms of CC-BY-NC-ND

Apart from the integration of external knowledge from diverse sources, the advantages of the multiagent AI approach are in the reduction of the need for human intervention, accessibility for nonexperts as well as interpretability [8]. Proposed "AtomAgents," a physics-aware multiagent framework given in work [8] comprises a team of agents constructing the core who collaborate to solve complex alloy design tasks with the help of a set of tools for different purposes. Besides that, certain tools that are implemented in AtomAgents, cover computations by atomistic simulations, knowledge retrieval from external sources, coding, plotting, and image analysis, making together LLM based framework for materials design and analysis [8].

3. CONCLUSION

Artificial intelligence is used in material science as well as in all spheres of life. As such, it opens up great possibilities in the alloys design, cost reduction and reduction of numerous experiments as well.

In order to fully use its potential, it is necessary to try to solve the challenges it brings in alloys design:

- development of standardized, open databases,
- combine AI with physically based models (CALPHAD, DFT, etc.),
- improve the interpretability of the model,
- establish a strong link between experiment and prediction.

In this way, artificial intelligence will not only serve as model for prediction itself, yet for understanding and optimizing complex phase transformations, structure and properties of modern alloys. It will be very helpful in education, for nonexperts as for industry, and for everyone who need knowledge and work in the area of alloys design and analysis.

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