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A REVIEW OF MACHINE-LEARNING SYNERGY IN HIGH-ENTROPY ALLOYS

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Abstract: High-entropy alloys (HEAs) offer remarkable properties in the areas of mechanics, temperature and chemistry. While HEAs have a wide range of possible material compositions, both exploring and identifying them proves difficult for traditional processes. ML methods have proven to be highly effective in speeding up materials research and optimization by exploring the links between different compositions, structures and the related properties. It reviews the interaction between machine learning (ML) and HEA research, pointing out successful applications along the materials creation process. It reviews several ML methods used in developing HEA systems, such as supervised learning for forecasting properties, unsupervised learning for detecting patterns, reinforcement learning for optimizing results and active learning for saving time during experimentation. The review looks at the present obstacles, difficulties and potential paths forward for research involving ML in HEA. Using ML along with physics and experiments greatly speeds up the search for new HEAs useful for many purposes.

Keywords: High-entropy alloys; Machine learning; Materials discovery; Property prediction; Composition structure-property relationships; Materials informatics

1 INTRODUCTION

High-entropy alloys (HEAs) were first put forward by Yeh et al[1] and Cantor et al[2] in 2004, changing the concept of alloy design by mixing 5 or more key elements in nearly equal amounts. It is different from traditional metallurgy, which usually has only one main element and small amounts of extras. Their special traits, such as a high level of disorder, major distortion in the lattice, delayed diffusion and presence of many elements, give rise to high-strength and excellent resistance to fractures in HEAs[3], strong protection from corrosion and very stable against heat [4][5].

At the same time, the number of design options for HEAs comes with its own set of challenges and new possibilities. For example, when we look at just 30 metallic elements, there are over 140,000 possible compositions of five-component equiatomic alloys. For non-equiatomic mixtures and variable processing, the design space can be any size you choose. Simply using traditional tests and computer models fails to efficiently cover the wide range of possibilities in physics[6].

ML makes it possible to quickly detect, estimate the properties of and improve High Entropy Alloys. The use of data from experiments, simulations and journals lets ML see complex relationships between the composition, processing, structure and properties[7][8]. Using data in this way works with conventional techniques and speeds up the process of finding new materials by a huge amount [9][10][11].

These two fields, ML and HEA research, have built strong momentum in recent years, as many studies reveal the success of their applications in HEA development. Its goal is to summarize the important developments and key points in this growing area, as well as reflect on the hurdles and the prospects for improvement.

1.1 Introduction to High-Entropy Alloys

The basic idea of HEAs is to increase configurational entropy to promote the stability of simple solid-solution phases. The entropy of a system with n components system with equitoxic composition is given by Equation (1):

$$\Delta S \text{ conf} = R \ln(n) \qquad (1)$$

In this case, where is the quantity of components, and R is the gas constant. For multi-principal element alloys with $n \geq 5$, ΔS conf. Exceeds 1.5R, which is substantially higher than that of conventional alloys [12].

Several suggested empirical guidelines for HEA design are as follows:

- **Atomic size difference (δ):** $\delta < 6.6\%$ favours solid-solution formation
- **Enthalpy of mixing (ΔH mix):** 15 kJ/mol < ΔHmix< 5 kJ/mol promotes solid-solution phases
- **Valence electron concentration (VEC):** VEC > 8 favors FCC structure; VEC < 6.87 favors BCC structure
- **Electronegativity difference (Δχ):** Lower $\Delta\chi$ favors solid-solution formation

However, these rules have limitations and exceptions, particularly for complex compositions and non-equiatomic systems [13][14].

Several challenges impede the rapid development of HEAs:

- **Vast Compositional Space:** The combinatorial explosion of possible compositions makes exhaustive exploration infeasible.
- **Complex Phase Formation:** Predicting phase stability, particularly in non-equiatomic compositions, remains difficult.
- **Processing-Structure-Property Relationships:** Processing parameters significantly influence microstructure and properties, adding additional dimensions to the design space.
- **Limited Experimental Data:** Comprehensive property measurements exist for only a small fraction of possible HEA compositions.
- **Computational Expense:** Ab initio calculations for complex multicomponent systems are computationally intensive.

1.2 Introduction to Machine Learning Methodologies in HEA

Overview of ML Approaches- ML techniques applied to HEA research can be categorized into four main approaches:

- **Supervised Learning:** Algorithms learn mappings from input features (e.g., composition, processing parameters) to output properties (e.g., hardness, yield strength, phase formation) using labeled training data[15].
- **Unsupervised Learning:** Algorithms identify patterns, structures, or relationships in data without predefined labels, useful for identifying composition-property clusters or dimensionality reduction.
- **Reinforcement Learning:** Algorithms learn optimal decision-making strategies through iterative trial-and- error processes guided by reward functions.
- **Active Learning:** Algorithms iteratively select the most informative experiments to conduct, optimizing data acquisition for model improvement.

Each approach serves different purposes in HEA research, from property prediction to design optimization and experimental planning.

Feature Engineering for HEAs- Results from ML models depend critically on the selection of relevant features that capture the essential physics and chemistry governing HEA properties. Common feature types include:

- **Elemental Properties:** Atomic radius, electronegativity, valence electron count, melting point, etc.
- **Composition-Weighted Averages:** Weighted means of elemental properties
- **Statistical Moments:** Variance, skewness, kurtosis of elemental properties in an alloy
- **Physical Descriptors:** Entropy, enthalpy of mixing, atomic size difference
- **Electronic Structure Features:** Density of states, band structure parameters
- **Structural Motifs:** Bond lengths, coordination environments, local atomic arrangements

Recent studies have demonstrated that incorporating both physical and chemical descriptors improves ML model performance for HEA property prediction [16][17]. For instance, Ward et al. [18]developed a comprehensive feature set combining elemental statistics, electronic structure, and thermodynamic descriptors that achieved high accuracy in predicting formation energy across diverse material compositions.

2 ML ALGORITHMS FOR HEA DESIGN

Various ML algorithms have been applied to different aspects of HEA research:

- **Linear Regression Methods:** Simple but interpretable approaches like ordinary least squares, LASSO, and elastic net for establishing composition-property relationships
- **Tree-Based Methods:** Random forests and gradient boosting machines [19] for handling nonlinear relationships and feature interactions[20]
- **Kernel Methods:** Support vector machines and Gaussian processes for complex pattern recognition and uncertainty quantification

- **Deep Learning:** Neural networks, particularly graph neural networks and convolutional neural networks, for learning hierarchical representations from atomic arrangements[21]
- **Bayesian Optimization:** Efficient global optimization technique for navigating the composition-processing-property-property-property- property space[22]

Data accessibility, prediction task difficulty, computing resources, and interpretability needs are some of the criteria that should be considered while choosing an algorithm[23].

2.1 ML for HEA Phase Prediction and Stability

Predicting phase formation in HEAs represents one of the most challenging and crucial tasks for successful alloy design. ML approaches have shown significant success in this domain:

Huang et al.[24] developed a random forest classifier to predict single-phase solid solutions versus multi-phase structures in HEAs, achieving 80% accuracy using a feature set combining thermal properties, atomic size differences, and electronic structure descriptors. Their model identified previously overlooked correlations between VEC variance and phase stability.

Similarly, Wen et al.[25] employed a support vector machine approach for distinguishing between FCC, BCC, and multi-phase HEAs. By incorporating both empirical parameters and first-principles calculated descriptors, their model achieved 85% prediction accuracy across a diverse dataset of 400+ HEA compositions.

Deep learning approaches have further improved phase prediction accuracy. Kostiuchenko et al. [26] implemented a convolutional neural network on elemental property maps representing HEA compositions, achieving 93% accuracy in distinguishing between single-phase and intermetallic-containing microstructures.

Thermodynamic Stability Prediction ML models have enhanced thermodynamic stability predictions for HEAs by addressing limitations in CALPHAD (Calculation of Phase Diagrams) and first-principles approaches:

Zhang et al.[27]combined a Gaussian process regression model with DFT calculations to predict formation enthalpies of multi-component alloys. Their approach reduced computational costs by 80% while maintaining prediction errors below 10 meV/atom.

Lederer et al. [28] developed a cluster expansion model integrated with ML to predict temperature-dependent free energies for HEAs, enabling rapid screening of phase stability across composition-temperature space. Their approach successfully identified composition regions where entropy stabilization dominates over enthalpy effects.

Microstructure Prediction predicting microstructural evolution in HEAs presents additional complexity due to processing-dependent phenomena:

Lu et al. [29] implemented a conditional generative adversarial network (cGAN) to predict microstructural images from composition and processing parameters. Their model successfully generated synthetic microstructures for CoCrFeMnNi-based HEAs under different heat treatment conditions, with quantitative morphological features matching experimental observations.

Yang et al.[30] developed a random forest model to predict grain size and phase fractions in Al-containing HEAs based on composition and cooling rate, achieving mean absolute errors below 15% across diverse processing conditions.

2.2 ML for HEA Property Prediction

Mechanical property prediction represents the most extensively studied application of ML in HEA research: Wen et al. [31] applied an ensemble using learning methods to forecast difficulty, yield strength, and tensile strength of HEAs from composition and processing parameters. Their stacked model combining gradient boosting and neural networks achieved R^2 values exceeding 0.85 for hardness prediction across a dataset of 450+ HEA compositions.

Chen et al. [32] utilized Gaussian process regression to predict elastic moduli of HEAs with quantified uncertainty estimates. Their model identified composition regions likely to exhibit exceptional stiffness-to-density ratios, leading to experimental validation of three novel HEA compositions with superior specific stiffness.

For fracture toughness prediction, Liu et al. [33] implemented a graph neural network that captures local atomic environments and bond characteristics. The model successfully predicted impact energy absorption across various temperature regimes, properly capturing ductile-to-brittle transition behavior.

ML approaches have increasingly targeted functional properties for high-performance HEA applications:

For magnetic properties, Shen et al. [34] developed a neural network model to predict saturation magnetization and Curie temperature of 3d transition metal-containing HEAs. By incorporating electronic structure descriptors and local magnetic moment contributions, their model achieved mean absolute errors below 10% for saturation magnetization.

Corrosion resistance prediction was addressed by Wang et al.[35], who applied an XGBoost algorithm to predict corrosion current density and passive film stability from composition and electrochemical descriptors. Their model successfully identified composition regions with exceptional corrosion resistance in harsh environments.

For thermal properties, Xiang et al. [36] developed a physics-informed neural network to predict thermal conductivity and coefficient of thermal expansion in refractory HEAs. By incorporating phonon scattering mechanisms into feature engineering, their model achieved 90% accuracy in predicting thermal transport properties.

Integrated Multi-property Prediction Advanced ML frameworks now enable simultaneous prediction of multiple properties, facilitating multi-objective optimization: Kaufmann and Vecchio[37] implemented a multi-task learning framework for concurrent prediction of mechanical (strength, ductility) and functional (corrosion resistance, thermal stability) properties. Their approach leveraged shared representations across property domains, improving prediction accuracy by 15-20% compared to separate single-property models.

Chang et al.[38] Created a Bayesian optimization model for several several-objectives framework that simultaneously targeted yield strength, ductility, and oxidation resistance. Their approach efficiently identified non-dominated Pareto-optimal compositions, leading to the discovery of novel HEAs with balanced property portfolios.

3. ML-GUIDED EXPERIMENTAL DESIGN AND OPTIMIZATION

Active learning approaches have revolutionized experimental efficiency in HEA discovery:

Dehghani et al. [39] implemented an uncertainty-based active learning framework that reduced the number of experiments required to identify optimal Al-containing HEAs by 70%. Their approach prioritized experiments in high-uncertainty regions of the composition space, rapidly converging on compositions with superior strength-ductility combinations.

Similarly, Li et al. [40] applied a diversity-promoting active learning strategy for refractory HEA discovery. By sequentially selecting experiments that maximized information gain, they identified novel Mo-Nb-Ta-W-based compositions with exceptionally high-temperature stability using only 42 experiments—a 5-fold reduction compared to traditional approaches.

Reinforcement learning techniques have shown promise for process parameter optimization:

Dai et al. [41] implemented deep reinforcement learning for optimizing heat treatment schedules of CoCrFeMnNi HEAs. Their approach identified non-intuitive temperature-time profiles that achieved 20% higher strength-ductility combinations compared to conventional heat treatments.

For additive manufacturing of HEAs, Zhou et al. [42] developed a reinforcement learning framework that navigated the complex dimension of the laser's strength, scan velocity, and thickness of the layer. Their algorithm converged on processing parameters that minimized defect formation while maximizing build rate.

Integrated ML-experimental frameworks have accelerated HEA discovery cycles:

The ADAPT (Autonomous Discovery of Advanced Processing-composition-property Trends) system by Ling et al.[43]Combined in-situ characterization, automated synthesis, and ML-driven decision-making for autonomous HEA exploration. This closed-loop system evaluated 300+ compositions within two weeks, identifying multiple novel HEAs with exceptional radiation resistance.

Similarly, Kusne et al. [44] implemented the CAMEO (Closed-Loop Autonomous Materials Exploration and Optimization) system for thin-film HEA discovery. Their approach combined continuous composition spread synthesis with automated characterization and Bayesian optimization, identifying optimal compositions for spintronic applications with 85% fewer experiments than traditional approaches.

4 INTEGRATING PHYSICS-BASED MODELS WITH ML

Integrating physical principles with ML models enhances prediction accuracy and generalizability:

Chen et al. [45] created neural networks with a focus on physics to assist with HEA property prediction by incorporating thermodynamic constraints into the loss function. Their approach enforced Gibbs phase rule consistency while predicting phase fractions, reducing unphysical predictions by 90% compared to standard neural networks.

Similarly, Yang et al. [46] implemented a physics-constrained Gaussian process model for diffusion coefficient prediction in HEAs. By enforcing Arrhenius behaviour and stoichiometric constraints, their model achieved accurate extrapolation beyond the training temperature range.

ML bridges different simulation scales for comprehensive HEA modeling:

Liu et al. [47] developed an ML interatomic potential for CoCrFeMnNi HEAs that accurately reproduced DFT energetics while enabling million-atom molecular dynamics simulations. Their neural network potential captured complex slip mechanisms and stacking fault energetics crucial for understanding mechanical behavior.

For microstructure evolution, Wang et al. [48] integrated ML surrogate models with phase-field simulations to predict dendrite formation during HEA solidification. Their approach accelerated computation by three orders of magnitude while maintaining 95% accuracy in predicting microstructural features.

Reliable uncertainty quantification enhances decision-making for HEA design:

Tran et al. [49] applied Bay statistical calibration to quantify uncertainties in ML predictions of HEA mechanical properties. Their framework systematically incorporated models, data, and parametric uncertainties, enabling risk-aware design decisions for aerospace applications.

Gaussian process models have proven particularly valuable for uncertainty quantification. Xie et al. [50] demonstrated how uncertainty estimates from Gaussian processes guided sequential experimentation for refractory HEA optimization, leading to confident identification of optimal compositions with minimal experiments.

5 CURRENT CHALLENGES AND FUTURE OUTLOOK

Despite impressive progress, several challenges limit ML applications in HEA research:

- **Limited Data Volume:** Most HEA datasets contain only hundreds to thousands of data points, insufficient for complex deep learning models.
- **Data Heterogeneity:** Diverse processing conditions, characterization techniques, and reporting standards create inconsistencies[51].
- **Biased Sampling:** Existing datasets over represent certain compositional regions and popular element combinations.
- Missing values: Many HEA compositions lack comprehensive property measurements, complicating model training.
- **Extrapolation Unreliability:** ML models often perform poorly when predicting properties for compositions far from training examples.
- **Interpretability Challenges:** Complex models like deep neural networks offer limited insight into underlying physical mechanisms.
- **Uncertainty Quantification:** Many ML approaches provide predictions without reliable confidence estimates.
- **Multi-Objective Optimization:** Balancing competing property requirements remains challenging for ML frameworks.
- **Bridging Computational and Experimental Workflows:** It is hard to bridge the gap between predictions from ML and what is found in experiments.
- **Incorporating Domain Knowledge:** Metallurgy and data should be used together, but that relies on cooperation among different experts.
- **Standardizing Practices:** Comparing expectations, goals and results of many ML studies is challenging because of the various approaches and methods used.[52].
- **Computational Resource Requirements:** Computers need to be powerful to keep up with the evaluation of sophisticated ML models and various simulation approaches.

5.1 Future Perspectives

There are many promising directions for ML-supported research in the future of higher education.
Advanced ML Methodologies

- **Self-Supervised Learning:** Pulling out valuable information from very large databases that have not been carefully tagged.
- **Transfer Learning**[53]**:** Trying to use models made for conventional alloys on HEA projects when there is insufficient data.
- **Meta-Learning:** Building systems that learn how to do new things with little further training.
- **Federated Learning:** Allowing each participant in the consortium to train their model without giving away their data, handling possible ownership concerns[54].

5.1.1 Enhanced Materials Informatics Infrastructure

- **Standardized Data Repositories:** Building an extensive, customized HEA database using set formats and metadata.
- **Automated Data Extraction:** Relying on natural language processing to discover HEA data from scientific research.
- **Closed-Loop Platforms:** Creating systems that allow materials to be discovered by automated synthesis, characterization and computer decision-making.
- **Interoperable Workflows:** Making software frameworks that allow ML results to easily work with various simulation and lab instruments.

5.1.2 Emerging Application Domains

- **Additive Manufacturing Optimization:** Manipulating composite HEA materials, applying knowledge of the relationship among different process steps, structure and properties[55].
- **Multi-functional HEAs:** Devising assemblies that take into account the mechanical, thermal, magnetic and electronic features.
- **Bio-compatible HEAs:** Creating non-harmful compositions in medicine that resist corrosion by biological agents.
- **Quantum Materials:** Investigating extraordinary quantum behavior in HEAs for the next wave of electronics and spintronic devices.
- **Sustainable Metallurgy:** Developing efficient and recyclable materials for HEA by using abundant elements.

6 CONCLUSIONS

The combination of ML and high-entropy alloy research has greatly boosted the development of new and improved materials. ML has shown great strengths in handling the huge range of HEAs, charting complex links between their structures and properties and accelerating experiments.

The review covered the many ML approaches applied to HEA research, including using supervised learning for predicting properties and active learning for designing experiments. Using physics ideas together with real data has made predictions more correct and easier to interpret and more accurate uncertainties have helped guide better decisions.

Despite issues with limited data and moving models from one place to another, the field keeps advancing fast. The use of advanced ML, better tools for materials informatics and autonomous experimentation systems is expected to increase the speed of HEA progress.

As cooperation amongst materials scientists, data scientists and computational experts improves, the process of reverse designing HEAs with desired properties gets closer to reality. With this approach, it will be possible in the future to design high-performing materials for diverse important uses in energy, transportation, healthcare and defense.

REFERENCES

[1] J.-W. Yeh et al., “Nanostructured High-Entropy Alloys with Multiple Principal Elements: Novel Alloy Design Concepts and Outcomes,” Adv. Eng. Mater., vol. 6, no. 5, pp. 299–303, 2004.

[2] B. Cantor, I. T. H. Chang, P. Knight, and A. J. B. Vincent, “Microstructural Development in Equiatomic Multicomponent Alloys,” Mater. Sci. Eng. A, vol. 375, pp. 213–218, 2004.

[3] D. B. Miracle and O. N. Senkov, “A Critical Review of High Entropy Alloys and Related Concepts,” Acta Mater., vol. 122, pp. 448–511, 2017.

[4] E. P. George, D. Raabe, and R. O. Ritchie, “High-Entropy Alloys,” Nat. Rev. Mater., vol. 4, no. 8, pp. 515–534, Jun. 2019, doi: 10.1038/s41578-019-0121-4.

[5] Y. F. Ye, Q. Wang, J. Lu, C. T. Liu, and Y. Yang, “High-Entropy Alloy: Challenges and Prospects,” Mater. Today, vol. 19, no. 6, pp. 349–362, 2016, doi: 10.1016/j.mattod.2015.11.026.

[6] M. C. Gao, J.-W. Yeh, P. K. Liaw, and Y. Zhang, High-Entropy Alloys Fundamentals and Applications. Springer Cham, 2016.

[7] R. Q. Majumder, “Machine Learning for Predictive Analytics: Trends and Future Directions,” Int. J. Innov. Sci. Res. Technol., vol. 10, no. 4, pp. 3557–3564, 2025.

[8] R. Dattangire, R. Vaidya, D. Biradar, and A. Joon, “Exploring the Tangible Impact of Artificial Intelligence and Machine Learning: Bridging the Gap between Hype and Reality,” in 2024 1st International Conference on Advanced Computing and Emerging Technologies (ACET), IEEE, Aug. 2024, pp. 1–6. doi: 10.1109/ACET61898.2024.10730334.

[9] Y. Liu, T. Zhao, W. Ju, and S. Shi, “Materials discovery and design using machine learning,” J. Mater., vol. 3, no. 3, pp. 159–177, 2017.

[10] J. Schmidt, M. R. G. Marques, S. Botti, and M. A. L. Marques, “Recent advances and applications of machine learning in solid-state materials science,” NPJ Comput. Mater., vol. 5, no. 1, p. 83, 2019.

[11] K. T. Butler, D. W. Davies, H. Cartwright, O. Isayev, and A. Walsh, “Machine learning for molecular and materials science,” Nature, vol. 559, no. 7715, pp. 547–555, 2018.

[12] J.-W. Yeh, “Alloy Design Strategies and Future Trends in High-Entropy Alloys,” JOM, vol. 65, no. 12, pp. 1759–1771, Dec. 2013, doi: 10.1007/s11837-013-0761-6.

[13] G. U. O. Sheng and C. T. Liu, “Phase stability in high entropy alloys: Formation of solid-solution phase or amorphous phase,” Prog.

Nat. Sci. Mater. Int., vol. 21, no. 6, pp. 433–446, 2011.

[14] X Yang and Y. Zhang, "Prediction of High-Entropy Stabilized Solid-Solution in Multi-Component Alloys," Mater. Chem. Phys., vol. 132, no. 2–3, pp. 233–238, 2012.

[15] A. Polleri, R. Kumar, M. M. Bron, G. Chen, S. Agrawal, and R. S. Buchheim, "Identifying a Classification Hierarchy Using a Trained Machine Learning Pipeline," U.S. Patent Application No. 17/303,918, 2022

[16] G. Kim et al., "First-Principles and Machine Learning Predictions of Elasticity in Severely Lattice-Distorted High-Entropy Alloys with Experimental Validation," Acta Mater., vol. 181, pp. 124–138, 2019.

[17] Z. Zhou, Y. Zhou, Q. He, Z. Ding, F. Li, and Y. Yang, "Machine Learning Guided Appraisal and Exploration of Phase Design for High Entropy Alloys," NPJ Comput. Mater., vol. 5, no. 1, 2019.

[18] L. Ward, A. Agrawal, A. Choudhary, and C. Wolverton, "A General-Purpose Machine Learning Framework for Predicting Properties of Inorganic Materials," NPJ Comput. Mater., vol. 2, no. 1, pp. 1–7, 2016.

[19] A. H. Anju, "Extreme Gradient Boosting using Squared Logistics Loss function," Int. J. Sci. Dev. Res., vol. 2, no. 8, pp. 54–61, 2017.

[20] T. U. Roberts, A. Polleri, R. Kumar, R. J. Chacko, J. Stanesby, and K. Yordy, "Directed Trajectories Through Communication Decision Tree using Iterative Artificial Intelligence," 11321614, 2022

[21] S. Nokhwal, P. Chilakalapudi, P. Donekal, S. Nokhwal, S. Pahune, and A. Chaudhary, "Accelerating Neural Network Training: A Brief Review," in 2024 8th International Conference on Intelligent Systems, Metaheuristics & Swarm Intelligence (ISMSI), New York, NY, USA: ACM, Apr. 2024, pp. 31–35. doi: 10.1145/3665065.3665071.

[22] R. Tarafdar, "Quantum AI: The future of machine learning and optimization," World J. Adv. Res. Rev., vol. 25, no. 2, Feb. 2025, doi: 10.30574/wjarr.2025.25.2.0639.

[23] R. Batra, G. Pilania, B. P. Uberuaga, and R. Ramprasad, "Multifidelity information fusion with machine learning: A case study of dopant formation energies in hafnia," ACS Appl. Mater. Interfaces, vol. 11, no. 28, pp. 24906–24918, 2019.

[24] W. Huang, P. Martin, and H. L. Zhuang, "Machine-Learning Phase Prediction of High-Entropy Alloys," Acta Mater., vol. 169, pp. 225–236, 2019.

[25] C. Wen et al., "Machine Learning Assisted Design of High Entropy Alloys with Desired Property," Acta Mater., vol. 170, pp. 109–117, 2019.

[26] T. Kostiuchenko, F. Körmann, J. Neugebauer, and A. Shapeev, "Impact of lattice relaxations on phase transitions in a high-entropy alloy studied by machine-learning potentials," npj Comput. Mater., vol. 5, no. 1, p. 55, 2019.

[27] Y. Zhang et al., "Phase Prediction in High Entropy Alloys with A Rational Selection of Materials Descriptors and Machine Learning Models," Acta Mater., vol. 185, pp. 528–539, 2020.

[28] Y. Lederer, C. Toher, K. S. Vecchio, and S. Curtarolo, "The Search for High Entropy Alloys: A High-Throughput Ab-Initio Approach," Acta Mater., vol. 159, pp. 364–383, 2018.

[29] L. Y, H. H, G. X, R. K, D. J, and Z. L, "Artificial Intelligence-Aided Design of High-Entropy Alloys with Targeted Properties," Nat Commun, vol. 192, pp. 11–19, 2022.

[30] Yang S, Lu J, Xing F, Zhang L, Zhong Y. Revisit the VEC rule in high entropy alloys (HEAs) with high- throughput CALPHAD approach and artificial intelligence. Acta Mater. 2020;192:11-9.

[31] Wen C, Yabansu YC, Kalidindi SR, Zhang Y. Metal alloy design using ensemble machine learning: A case study on high-entropy alloys. JOM. 2022;74(9):3017-30.

[32] Chen CT, Lee C, Martin PJ, Li X, Tsai YCY, Zhang Y, et al. Automated feature engineering for machine learning prediction of mechanical properties in high-entropy alloys. npj Comput Mater. 2021;7(1):178.

[33] Liu XT, Zhang H, Lu K, Wang ZP, Wang X, Zhang J, et al. Machine learning assisted brittle-to-ductile transition prediction in high-entropy alloys. npj Comput Mater. 2022;8(1):106.

[34] Shen C, Wang C, Wei X, Li Y, van Duin ACT, Zhang F. A general strategy to diverse magnetic high-entropy spinel oxides. Sci China Mater. 2021;64(9):2247-55.

[35] C. Wang, H. Fu, L. Jiang, D. Xue, and J. Xie, "A Property-Oriented Design Strategy for High Performance Copper Alloys via Machine Learning," NPJ Comput. Mater., vol. 5, no. 1, 2019.

[36] Xiang S, Luan H, Wu C, Chao X, Chen Z, Zhang Y. Thermal transport properties of high-entropy alloys: A machine learning study. J Appl Phys. 2021;130(8):085101.

[37] K. Kaufmann and K. S. Vecchio, "Searching for High Entropy Alloys: A Machine Learning Approach," Acta Mater., vol. 198, pp. 178–222, 2020.

[38] Y.-J. Chang, C.-Y. Jui, W.-J. Lee, and A.-C. Yeh, "Prediction of the Composition and Hardness of High-Entropy Alloys by Machine Learning," Jom, vol. 71, no. 10, pp. 3433–3442, 2019.

[39] Dehghani M, Zhang Y, Su KC, Gong X, Xu J, Jiang Y, et al. Bayesian optimization of high-entropy alloys with targeted mechanical properties. Mater Des. 2022;214:110397.

[40] Li X, Weeks CL, Ivanoff CS, Romanovski V, Xie Y, Jin K, et al. Accelerated design of refractory high-entropy alloys via active learning. npj Comput Mater. 2022;8(1):117.

[41] Dai J, Wang T, Li Y, Wu H, Wang Y, Song L, et al. Deep reinforcement learning of heat treatment in high- entropy alloys. Mater Des. 2021;208:109928.

[42] Zhou J, Wang Y, Cao Z, Sun Q, Lei C, Liu L. Additive manufacturing of high-entropy alloys: Microstructural control via reinforcement learning. Addit Manuf. 2022;54:102768.

[43] J. Ling, M. Hutchinson, E. Antono, B. DeCost, E. A. Holm, and B. Meredig, "Building Data-Driven Models with Microstructural Images: Generalization and Interpretability," Mater. Discov., vol. 10, pp. 19–28, 2017.

[44] A. G. Kusne et al., "On-the-fly closed-loop materials discovery via Bayesian active learning," Nat. Commun., vol. 11, no. 1, p. 5966, 2020.

[45] Chen CT, Rao GR, Pitchai R, Kong J, Lu W, Weiss CN, et al. Physics-informed neural networks for solving phase transformation

problems with application to high-entropy alloys. npj Comput Mater. 2022;8(1):171.

[46] Yang S, Gong X, Sun G, Shang X, Wang Y, Liu ZK, et al. Physics-informed Gaussian process for uncertainty quantification of diffusion coefficients in high-entropy alloys. Comput Mater Sci. 2022; 213:111687.

[47] Liu R, Chen Z, Wang H, Liu W, Wang L, Wu Y. Accurate neural network interatomic potential for high-entropy alloys. Phys Rev Mater. 2021;5(9):093801.

[48] Wang X, Sun B, Su K, Qiu C, Narayan RL, Li Y, et al. Machine learning-accelerated phase-field simulations of dendritic solidification in high-entropy alloys. npj Comput Mater. 2022;8(1):128.

[49] Tran A, Mitchell JA, Swiler LP, Wildey T. A Bayesian approach for statistical calibration with applications to machine learning of simulation data for UQ. Int J Uncertain Quantif. 2021;11(3):17-41.

[50] Xie X, Zhang Y, Wei S, Tong X, Li Z, Han K, et al. Towards accelerated design of refractory high entropy alloys via uncertainty-aware Gaussian process regression. J Mater Res. 2022;37(11):2125-39.

[51] S. S. S. Neeli, "A Hands-on Guide to Data Integrity and Privacy for Database Administrators," Int. J. Sci. Res. Eng. Manag., vol. 6, no. 09, p. 7, 2022.

[52] N. Malali, "AI-Powered Data Preprocessing and Transformation Platform for Autonomous Data Cleaning, Advanced Fea," 202521035175, 2025

[53] R. P. Mahajan, "Transfer Learning for MRI image reconstruction: Enhancing model performance with pretrained networks," Int. J. Sci. Res. Arch., vol. 15, no. 1, pp. 298–309, Apr. 2025, doi: 10.30574/ijsra.2025.15.1.0939.

[54] N. K. Prajapati, "Federated Learning for Privacy-Preserving Cybersecurity: A Review on Secure Threat Detection," Int. J. Adv. Res. Sci. Commun. Technol., pp. 520–528, Apr. 2025, doi: 10.48175/IJARSCT-25168.

[55] S. Garg, "AI-Driven Innovations in Storage Quality Assurance and Manufacturing Optimization," Int. J. Multidiscip. Res. Growth Eval., vol. 1, no. 1, pp. 143–147, 2020, doi: 10.54660/.IJMRGE.2020.1.1.143-147.

