Journal of Nuclear Materials 559 (2022) 153462

Contents lists available at ScienceDirect

Journal of Nuclear Materials

journal homepage: www.elsevier.com/locate/jnucmat

Application of machine learning in understanding the irradiation damage mechanism of high-entropy materials

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ARTICLE INFO

Article history:
Received 9 September 2021
Revised 3 December 2021
Accepted 4 December 2021
Available online 5 December 2021

Keywords:
high-entropy materials
Machine Learning
Irradiation damage
kinetic Monte Carlo
Multi-scale simulation
defect evolution

ABSTRACT

The concept of high entropy materials (HEMs) provides a fertile ground for developing novel irradiation-resistant structural materials. In HEMs, the vast and complicated configurational space induced by extreme disorder poses grant challenges to understanding defect dynamics and evolution. Machine learning (ML) techniques, which can exploit implicit relationships between diverse descriptors and observations, exhibit great potential in uncovering the governing factors for irradiation damage and modeling local environment dependence of defect dynamics. Herein, three applications of ML in understanding radiation damage in HEMs are summarized and discussed, including ML-based irradiation response prediction, ML-based interatomic potential development, and ML-informed defect evolution.

1. Introduction

The development of high-entropy alloys has fundamentally changed the paradigm of materials design [1]. Inspired by the concept of entropy stabilization, a wide class of high entropy materials (HEMs) besides HEAs, including high entropy ceramics [2], high entropy metallic glass [3], and high-entropy nanoparticles [3] with remarkable properties, have been successfully discovered. HEMs usually consist of multiple components with quasi-equimolar ratios, leading to extreme chemical disorder in the structure. It has been found that almost all the extraordinary properties of HEMs are exclusively related to the disordered states, such as excellent mechanical performance overcoming the strength-ductility tradeoff [4] and promising irradiation resistance [5–7]. Therefore, tuning disorder has become a profitable strategy to improve the performance of HEMs. A fundamental understanding of how the disorder affects the irradiation response of HEMs is the key to the realization of radiation-tolerant multicomponent materials for nuclear applications.

The chemical disorder in HEMs originates from the random arrangement of different elemental species all at high concentrations. As such, defect properties, such as defect formation and migration, are strongly heterogeneous depending on the local atomic environments. It has been shown that such local environment dependence of defect properties may be complicated without apparent relationships. In particular, such dependence could extend to several nearest neighbor (NN) shells. As a consequence, though some attempts have been made to correlate defect properties with its local structures [8], there is still no general framework through which defect behavior can be assessed under highly variable atomic environments. As microstructure changes under irradiation are mainly driven by defect evolution, our ability to understand and predict defect evolution under the influence of chemical heterogeneity is extremely crucial.

In recent years, machine learning (ML) has played increasingly important roles in material science [9]. Built upon the data from either experiments or simulations, a well-trained ML model can be used for the discovery of new phases and for the prediction of properties under unknown conditions. Considering the spatial heterogeneity of defect evolution in HEMs, ML is an ideal tool to exploit the hidden connections between the irradiation performance and inherent disorder. Here in this contribution, the application of ML in understanding the radiation performance of HEMs is reviewed and envisaged. As this is a new area, there are only a few available studies on the direct application of ML in HEMs. In terms of the complex atomic environments governed defect process, HEMs share structural similarities to traditional alloys. Indeed, even in dilute binary alloys, the possible combinations of atomic configurations surrounding a defect are numerous. Thus, some developed methodology in metallic alloys is still applicable in the field of HEMs, and our discussions will be mainly based on published research on traditional alloys. We outline three directions for the application of ML in comprehending irradiation damage mechanisms of HEMs, as illustrated in Fig. 1. Specifically,

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https://doi.org/10.1016/j.jnucmat.2021.153462
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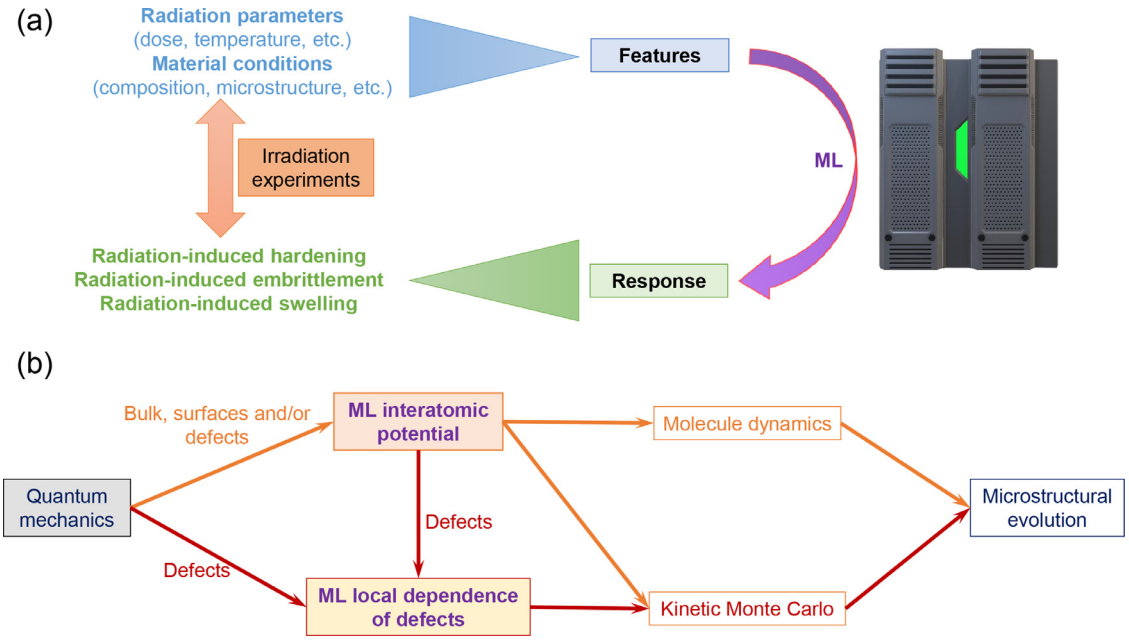

Fig. 1. Overview of applications of ML in understanding irradiation performance of HEMs. Three applications are delineated, including ML prediction of irradiation response (a), ML-based interatomic potential development, and ML description of local environment dependence of defects (b).

we will delineate one application of ML in experimental studies and two in theoretical modeling. Our perspectives on the challenges and future research opportunities relating to ML techniques in HEMs are presented in the last section.

2. ML-based prediction of irradiation response

Irradiation-induced materials degradation, in the order of temperature, include hardening and embrittlement (<0.4 T_m), precipitation (0.3–0.6 T_m), creep (<0.45 T_m), volumetric swelling (0.3–0.6 T_m), and He embrittlement (>0.5 T_m), where T_m denotes melting temperature [10]. These phenomena could lead to mechanical failure of structural materials and pose threats to the operation of nuclear reactors. Therefore, understanding and predicting the occurrence of these detrimental effects is of utmost importance. Generally, these effects depend on the states of materials and environmental conditions. By establishing the connections between these descriptors and experimentally measured irradiation response, an ML model can be built and used to make predictions for given new materials and environmental variables, as illustrated in Fig. 1(a). The major hurdle for such practice is the acquisition of enough data since the success of ML hinges on the quality and broadness of input data in the interconnected parameter space.

For traditional nuclear materials such as steels, ML has been applied to predict their irradiation response with reasonable accuracy. For instance, ML can predict the irradiation-induced embrittlement and hardening of reactor pressure vessel (RPV) steels [11–14], the ductile to brittle transition temperature of martensitic steels [15], and the onset dose for volume swelling in metallic materials [16]. In addition, ML has been used to predict the thermal conductivity and fission gas release in nuclear fuels [17,18]. Based on the obtained ML model, the relative importance of input variables can be evaluated, especially the metallic elements with predominating roles. These applications are exemplified in Fig. 2, in which satisfactory prediction accuracy is found in spite of the large spread in the experimental data.

The application of ML to predict the irradiation response of HEMs is yet to be demonstrated. It is foreseen that data availability would be a major limiting factor for building ML models, as irradiation study of HEMs is still in its infancy. Incorporating with published results on traditional materials is indispensable. Such ML models, once developed, will be able to shed light on the role of chemical complexity on the irradiation performance of HEMs by identifying the most contributing elements and their optimal concentrations. Considering the immerse phase space inherent in HEMs, the ML model can fast screen candidate HEMs with promising irradiation response, thus significantly reducing the time and expense for HEM development. In this regard, an integrated effort worldwide would be necessary to accumulate data for a robust and predictive ML tool.

3. ML-based interatomic potentials for defect dynamics

The microstructure evolution under irradiation is controlled by the dynamics of defects introduced by the energetic particle bombardment. Therefore, understanding defect dynamics under the influence of chemical disorder in HEMs is critical to evaluate their irradiation performance. An accurate description of the defect process relies on a high-fidelity account of interatomic interactions. Although electronic structure calculations, such as density-functional theory (DFT), can generally provide quantum mechanical accuracy, it is restricted by the time and spatial scale of the simulation that can be performed. By virtue of ML models, it is possible to transfer the accuracy obtained in DFT to larger scales by establishing ML-based interatomic potentials (IAPs).

IAPs lie in the heart of molecular dynamics (MD) simulation, which is a powerful method to probe the microscopic process in materials. Through IAPs, key parameters required for mesoscale and continuum materials modeling can be easily calculated. In principle, the role of IAPs in MD is to provide the information of energy and atomic forces for any atomic configurations, based on which the system evolves according to the Newton's second law. IAPs for HEMs with multi-principal components are highly challenging to fit with empirical formalisms due to the high-dimensional configurational space, which greatly limits the applications of MD in simulating HEMs. In fact, currently, MD studies on irradiation resistance of HEMs are only focused on binary and ternary alloys due to the unavailability of suitable IAPs.

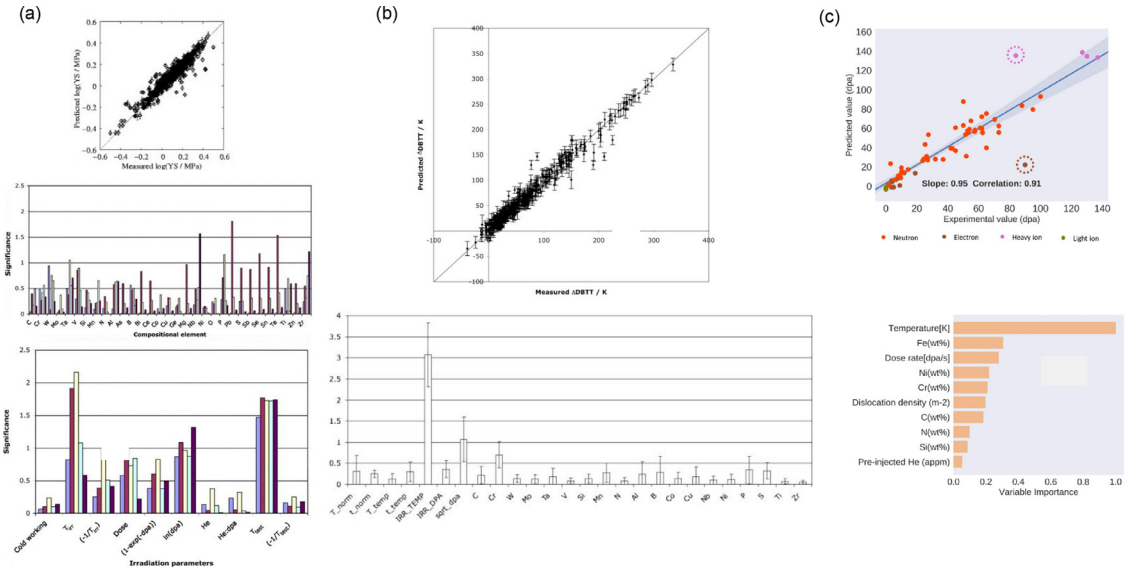

Fig. 2. ML prediction of (a) irradiation-induced hardening [14], (b) irradiation-induced Charpy ductile-brittle transition temperature [15], and (c) irradiation-induced onset dose for volumetric swelling[16]. Based on the ML model, the relative feature importance is given in the second row, which includes irradiation parameters and material composition.

In the spirit of ML, IAP can be viewed as a well-trained model for energy and force predictions. Such an ML model should be able to represent the potential energy landscape defined by various atomic configurations. Usually, the model is constructed based on an immerse reference database produced from DFT calculations, as schematically shown in the upper part of Fig. 1(b). Specifically, staring from quantum mechanics calculations, the properties of bulk phases, surfaces and defects can be obtained, which forms a large database containing energies and forces from different structures. The database can then be used for ML IAP development, based on which molecular dynamics can be established to study microstructural evolution. Thanks to high-dimensional regression models provided by ML, IAPs for multicomponent materials can be built, which are capable of describing a wide variety of material properties depending on the training data. Presently, there are various versions of ML IAPs, such as Gaussian approximation potential (GAP) [19], Behler-Parrinello neural network potentials (BPNNPs) [20], spectral neighbor analysis potentials (SNAPs) [21], and deep learning potentials (DLPs) [22]. The fundamentals of ML IAPs have been addressed by recent reviews [9,23–25]. Here, only the features pertinent to the study of radiation damage are discussed.

Irradiations from high-energy particles can bring atoms close enough in a short time. Hence, the short-range repulsive interactions among atoms are crucial for modeling the irradiation damage process. Usually, the repulsive force is calculated by the universal screened Coulomb Ziegler-Biersack-Littmarck (ZBL) formula [26]. Thereby, it is necessary to join the ML IAPs trained from the DFT database for equilibrium structures with the short-range ZBL potential. Indeed, superimposing ZBL with the ML IAP (Fig. 3(a)) reproduces well the angular-dependent threshold displacement energy for W, as provided in Fig. 3(b) [27]. To overcome the ambiguities in the transition region between ZBL and ML IAP, an all-electron database may be established to accurately account for the interactions over the whole distance.

The IAPs for modeling radiation damage should be able to describe not only different bulk phases, but also the diverse defect forms that may appear under irradiation, both of which are complicated due to the chemical complexity of HEMs. As the performance of ML IAPs exclusively depends on the given training set, enough defect configurations should be sampled in the database for constructing ML IAPs. This usually overwhelmingly increases the computational burden for DFT calculations due to the defect-induced symmetry breakdown in the lattice. Consequently, establishing such a database for multicomponent systems is an exceedingly intricate and challenging task. Hence, while general-purpose ML IAPs are extremely useful, it is reasonable to have tailored IAPs designed for special needs. For instance, with the purpose of Atomistic kinetic Monte Carlo (AKMC) simulation of thermal aging for Fe-Cr and Fe-Cu alloys, Castin et al. [28] fitted rigid-lattice high-dimensional neural network potentials (NNPs) based solely on DFT-calculated point defect migration energies. The introduction of such NNPs provides a flexible scheme to transfer the information of accurate static migration barriers with DFT accuracy to the MC scale with acceptable computational cost. Very recently, Byggmästar et al. developed an ML IAP for BCC MoNbTaVW [29] on the basis of the developed ML IAPs for its constituent pure refractory elements [27,30] within the GAP framework. The potential is designed to study elemental segregation and radiation damage in the studied HEM, as exemplified in Fig. 3(c). However, in the training dataset of this potential, defect configurations up to 5 vacancies and self-interstitials are considered only in the pure elements and in equiatomic random MoNbTaVW alloys. As a result, it may become less reliable when non-equiatomic compositions or constituent binary, ternary, and quaternary alloys are present under non-equilibrium conditions.

Compared to irradiation-induced defect studies, ML IAPs for dislocation studies are relatively abundant. The properties of dislocations, such as their core structures and mobilities, are related to mechanical deformation and failure, which is a focus of research for HEMs. For example, NNP IAPs are established for Al-Mg-Si [31] and Al-Cu [32] to study the mechanical behavior, crack propagation, and precipitate process in Al. In the database, diverse interface structures with different orientations between precipitates and the Al matrix are included, which enable high-fidelity predictions of dilute solid-solution energetics and precipitate/matrix interfaces. A SNAP IAP is constructed for NbMoTaW [33] to study its strengthening mechanism. Besides the bulk properties included in the DFT dataset, surface structures of the elemental systems are considered, enabling the study of elemental segregation in the bulk and near dislocations and grain boundaries.

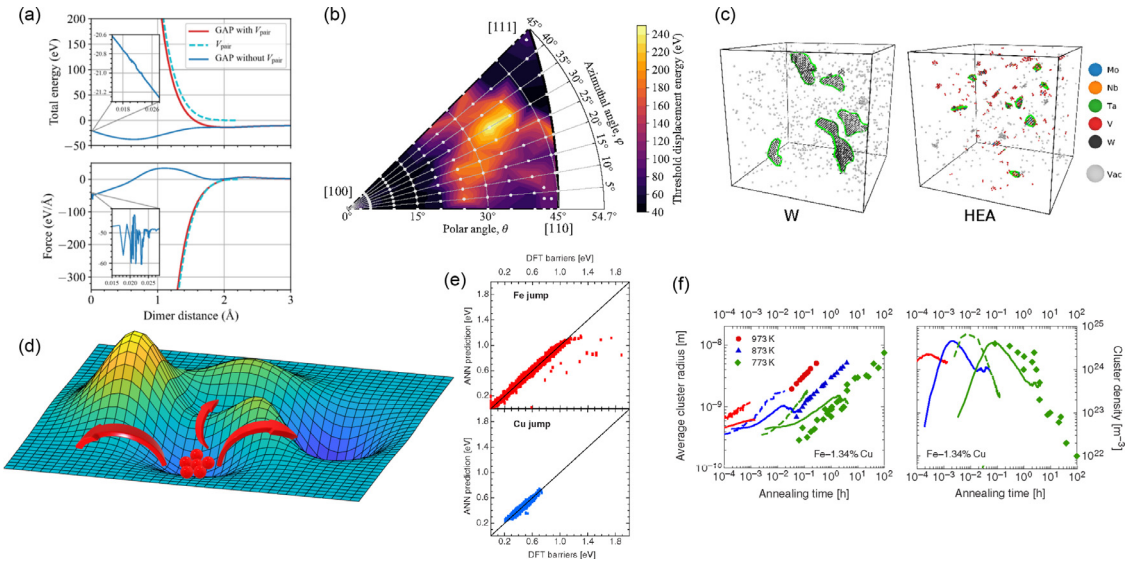

Fig. 3. ML in understanding defect evolution. The first row shows the energy and force given by ML IAPs combined with short-range repulsive interactions [27], which can be used to simulate radiation damage such as threshold displacement energy [27] and defect structures [29]. The second row explains the rough energy landscape for defect motion in HEMs, and ML can be used as a tool to model the local atomic environment dependence of defect migration [34].

Overall, ML provides a universal tool to model interatomic interactions for HEMs, where empirical formula may be insufficient to describe the complex interactions due to chemical complexity. The major obstacle is the acquisition of a DFT database that can encompass the huge configurational and compositional space, especially when defects are involved. However, there is also a need to refine ML models for HEMs since there are a wide variety of ML algorithms with different mathematical formalisms. In addition, calculation speed is also a factor that is worth considering when adopting ML IAPs, especially for irradiation damage simulations which often involve a large number of atoms, since ML IAPs are generally slower than analytical IAPs.

4. ML-based defect energetics for defect evolution

Long-term defect evolution controlled by thermally-activated events is commonly beyond the MD scale, which calls for higher scale techniques, such as kinetic Monte Carlo (kMC). For microstructure changes driven by the diffusion process, the most crucial factor is the defect energetics, which is responsible for defect-mediated mass transport. In HEMs, the chemical complexity of local atomic configurations induces salient heterogeneity in defect energetics (Fig. 3(d)). It is widely accepted that DFT calculations can provide a high-fidelity description of defect properties, though at a high computational cost. Available DFT calculations have shown that defect energetics strongly depends on local atomic environments in HEMs, and defect formation and migration energies exhibit broad distributions [8,35–38]. However, a quantitative correlation between defect energetics and their local environments remains elusive. A predictive tool will be helpful to fast screen and evaluate defect properties in HEMs by circumventing expensive DFT calculations on the vast compositional space.

The relations between defect energetics and local atomic environments are complicated in the configurational space. Using ML high-dimensional regression models, it is possible to map the local environments of defects onto their energetics. If the local environment dependence of defects can be captured by a well-trained ML model, defect properties could be easily assessed. The early works of Djurabekova et al. [39] and the following development of Castin et al. [28,34,40–42] unequivocally demonstrate the viability of ML models in describing the local atomic environment dependence of defect energies in RPV alloys. Specifically, it is found that artificial neural networks (ANN) can predict vacancy migration energies under different local atomic environments. Motivated by irradiation-induced embrittlement in RPV steels, the considered alloys are mainly Fe-based alloys, including FeCu, FeCr, FeCuNi, FeNiCr, and even FeCuNiMn. A large database is generated within carefully designed local atomic environments through the nudged elastic band method using an empirical IAP. The typical size of the training dataset, i.e., migration barriers here, is 30 000–100 000. It is seen that, with the development of sophisticated ML models, the accuracy and capability of ML are greatly expanded.

As ML training typically requires a large database to encompass the immerse configurational space, most studies rely on empirical IAPs to generate the training data. Replacing IAPs with accurate DFT calculations would considerably enhance the physical reliability of the defect database, but at the cost of higher computational intensity. Castin et al. [28] demonstrated that an ANN model could be built with DFT-derived migration barriers in FeCu and FeCr, which greatly improves the description of thermal aging experiments, as displayed in Fig. 3(e) and 3(f). The database includes the migration barriers for 2000 single-vacancy and 5600 self-interstitial atoms calculated at different local atomic configurations, with extra caution taken to select representative environments that may be encountered in the considered problem.

It can be expected that the above-mentioned methodology can be transferred straightforwardly to HEMs. In fact, some alloys that are touched in the works of Castin et al. can already be viewed as HEMs, such as FeCuNiMn [41]. However, with increasing chemical complexity, the configurational space experienced by the defect (vacancy or interstitial) goes up remarkably, which would require a larger database for an ML model to get a satisfying prediction ability. This seems computationally unmanageable at the *ab initio* level.

Recently, another type of ML model, namely support vector regression (SVR), has been applied to predict vacancy formation and migration energies in the Ni-Fe-Cr-Co-Cu five-component HEAs [43]. The model is built from the energetic database calculated from their constituent binary compositions based on empirical IAPs. It is found that accurate predictions can be achieved with a reduced training dataset, as low as ten data points from each binary composition. The results are encouraging, considering that

only hundreds of calculations are needed, which can be easily performed with DFT. However, even for a single vacancy in a binary alloy, there still exist numerous local atomic configurations, as demonstrated by Castin et al. [28,34,40–42]. It is not immediately clear how to choose suitable local environments from the binary constituents to be included in the training set. In addition, only a single vacancy is considered here. Whether the observed trend still holds for other types of defects, especially for interstitial with an anisotropic strain field, is still to be studied.

Besides point defects, early results have also suggested that ANN models can represent the local environment dependence of defect clusters [44]. For example, the migration barriers of Cu vacancy clusters V_n until $n = 6$ in Fe are predicted from ANN models, with the aim of obtaining their diffusion properties. The challenge for ANN regression for clusters is the higher configurational complexity in the local environments. As a result, the prediction accuracy is not as good as that for point defects. ANN models have also been applied with reasonable accuracy to describe the local environment dependence of defect energies under the influence of other structural features, such as grain boundaries [40,45] and surfaces [46].

The knowledge of defect energetics, especially migration barriers, allows studying the diffusion-controlled process governing microstructure evolution through versatile kMC algorithms. In kMC, the transition rates for all possible events are given by migration barriers, changing with varying local environments during defect evolution. Since the well-trained ANN models can make accurate predictions on migration barriers at different local environments, they can act as on-the-fly barrier predictors in kMC algorithm, as illustrated in the lower part of Fig. 1(b). The local atomic environment dependences of defects are first established by quantum mechanical calculations; they are then fed into ML ANN models for training and prediction, based on which kinetic Monte Carlo simulations are performed to monitor microstructural evolution under irradiation. The combination of ANN and kMC has proved to be successful, through which the simulated precipitation process of Cu in RPV steels is consistent with the thermal annealing experiment [28,34,42]. In particular, with the DFT-informed ANN model, the precipitation curve nearly matches perfectly with experimental observations [28].

It is demonstrated that paring ML with kMC is a powerful tool to investigate long-term defect evolution. Particularly, it can transfer knowledge gained at the DFT level to kMC scale. For HEMs, the vast configurational space makes it highly challenging to establish a DFT-based defect database. Hence the IAPs constructed by ML may be used to replace demanding DFT calculations. For this purpose, however, it is necessary to carefully design the local configurations that enter the IAP training database. With the well-established database, possible short-range order, typically found in HEMs [47], can be considered consistently by varying local environments.

5. Perspective and conclusion

HEMs represent a novel class of materials that greatly expand the material design space. The chemical complexity in HEMs endows them exceptional mechanical and irradiation performance, but at the same time, making it intricate to pinpoint the dominating factors in influencing their properties for rational design. Considering the vast compositional and configurational space, the conventional methodology is particularly struggling to capture the dependence of various observations on the underlying disorder states in HEMs. ML, as a unique tool that can mine implicit relationships among the target values and given descriptors, is particularly suitable for understanding and guiding irradiation-resistant HEM design.

The development of novel HEMs with improved irradiation tolerance rests on the integrated endeavor from both experimental and computational sides. As radiation damage is a multi-scale phenomenon, understanding their irradiation damage mechanism requires a thorough assessment of defect dynamics at hierarchically different scales, as well as how these processes at differing spatial and time scales couple together to determine the material performance. For multi-scale processes, it is always a challenge to link different models that bridge over different scales. This is particularly the case for HEMs bearing extreme chemical heterogeneities. In this sense, ML can be used to represent the feature of chemical complexity at lower scales, on which parameterization of higher-scale models can be built without loss of local structural information.

Based on the above considerations, three application realms of ML for nuclear materials exploitation based on HEMs are envisaged, including ML-based irradiation response prediction, ML-based IAP development, and ML-informed defect evolution, which are promising and feasible according to preliminary attempts. However, all these tasks depend on the availability of an extensive dataset within the considered parameter space, either from experiments or electronic structure calculations, as ML models generally rely on interpolation between known reference data. The data required are the correspondence between irradiation response and irradiation parameters and materials conditions. For ML-based defect evolution modeling, the data will be local atomic environment dependence of defect energetics. For ML purposes, the consistency of data is extremely crucial for high-fidelity training and prediction. Therefore, it is highly desirable that the conditions under which the data is generated should be enumerated in detail in order to fully interpret the reported dataset. Toward better interpretability, the black-box nature of the ML approach calls for rigorous evaluation of the physical foundations of ML predictions. Assisted with physical knowledge aggregated in the community over generations, it is expected that ML will become an indispensable ingredient in the future R&D for irradiation-tolerant materials with multiple principal components.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT authorship contribution statement

Shijun Zhao: Conceptualization, Investigation, Writing – review & editing.

Acknowledgement

This work was supported by the Research Grants Council of Hong Kong (Nos. 21200919 and 11200421), and City University of Hong Kong (No. 9610425).

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