Neural-network model for force prediction in multi-principal-element alloys

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Atomistic simulations can provide useful insights into the physical properties of multi-principal-element alloys. However, classical potentials mostly fail to capture key quantum (electronic-structure) effects. We present a deep 3D convolutional neural network (3D CNN) based framework combined with a voxelization technique to design interatomic potentials for chemically complex alloys. We highlight the performance of the 3D CNN model and its efficacy in computing potentials using the medium-entropy alloy TaNbMo. In order to provide insights into the effect of voxel resolution, we implemented two approaches based on the inner and outer bounding boxes. An efficient 3D CNN model, which is as accurate as the density-functional theory (DFT) approach, for calculating potentials will provide a promising schema for accurate atomistic simulations of structure and dynamics of general multi-principle element alloys.

INTRODUCTION

Multi-principal-element alloys, often called high- and medium-entropy alloys (HEAs/MEAs), continue to draw significant attention due to their remarkable mechanical behavior. However, the HEA design space is impractically large to explore mechanical properties of all possible compositions using experiments or first-principles calculations due to limitations on system size. On the other hand, computational modeling by atomistic simulations, especially for the sub-micron length processes, has not been progressed due to the absence of well-defined force fields to describe interatomic interactions.17–19 An interatomic potential function refers to the mathematical equation that provides a direct functional relationship between the configurations, positions, and potential energy of a group of atoms. Analytical potentials provide a simpler, direct, closed-form relation between the molecular configurations and their potential energy, which facilitates a quick energy calculation, but they are usually derived by introducing physical approximations.20 These potentials represent a necessary compromise between efficiency and accuracy, given that the essential characteristics of the atomic interactions are reasonably described. In molecular-dynamics simulations,21 force-field functions, such as the embedded atom method (EAM),22 are available for a limited set of elemental-combinations in HEAs and can be employed to describe the self and cross-interactions between different participating species. Atomistic simulations that utilize suitable interatomic potentials to describe the atomic interactions can easily overcome the shortcomings of first-principles theory and connect directly to experiments. However, there are not many attempts to address issues related to interatomic potentials for multi-principal element alloys such as HEAs.23 Notably, the absence of a general scheme provides an opportunity for designing reliable, useful, and robust interatomic potential functions. Machine-learning models can provide one such avenue for the accelerated design of interatomic potentials. Although extensively explored using machine learning, the design of interatomic potentials for atomistic simulations was mostly focused on simple elemental or binary systems.20,24–25 Also, the volumetric nature of the atomic feature descriptors (i.e., position of atoms, interatomic distances, etc.) makes the machine-learning methods more effective.20,25 If properly trained, a machine-learning-based interatomic potentials can provide the accuracy of density-functional theory (DFT) based methods.20,25

Here, we present a deep-learning convolutional neural network (CNN) model seeded with data from density-functional theory (DFT) based ab initio molecular dynamics (AIMD) simulations to develop interatomic potentials for HEAs. These potentials utilize CNN machine-learning models to construct direct functional correlations between the configuration, atomic position, energy, and forces20,24 using a consistent set of atomistic data.20,24,25 DFT-AIMD-based machine-learned potentials will enable faster evaluation of potentials, especially for large MD or Monte Carlo (MC) simulations general applicability to all possible interactions within a system containing various atomic species, and high-predictive accuracy comparable to DFT methods. These ideas were tested on a ternary TaNbMo MEA within a 54-atom random configurational model, created from Hybrid Cuckoo Search optimized Super-Cell Random Approximates (SCRAPs).20 Although any sized cell could be considered, it is limited by the cost of the DFT data generation. Our 3D CNN model shows great promise for developing alternate approaches for the design of atomistic potentials.
FIG. 1. Convolutional Neural Network (CNN) architecture was used to learn the relationship between the potential energy surface and the atomic coordinates of the alloy cell. The CNN architecture primarily consists of convolutional layers followed by max-pooling layers and one fully-connected layer at the end succeeded by the output.

METHODS

Deep Convolutional Neural Networks: Data encountered in real life often involves learning from three-dimensional (3D) data. Naturally, this has been a major area of deep learning research, where 3D CNNs were used to learn from 3D data. One of the earliest works on using 3D CNNs was for object detection (VoxNet) using a 3D voxelized geometry of simple objects (such as a bed or a chair)\textsuperscript{47,48} Since then, this idea has been exploited in several areas, such as object detection from point cloud data obtained using LIDARs\textsuperscript{49} engineering data used in design for manufacturing applications\textsuperscript{50} material microstructures synthesis applications\textsuperscript{51,52} and rendering smooth three dimensional graphics\textsuperscript{53}

A deep neural-network consists of several layers of connections forming one network, which takes an input \(x\) and produces an output \(y\). Each connecting layer \((l_i)\) in the network can be represented as \(y_{li} = \sigma(W_{li} \cdot x_{li} + b_{li})\), where \(\sigma(...)\) represents a non-linear activation function, \(W_{li}\) and \(b_{li}\) are the weights and biases, respectively, for connecting the input neurons \((x_{li})\) to the output \((y_{li})\) neurons. The connections could be as simple as a dense connection between every input neuron and output neuron in the layer. However, all connections in a dense connection layer may not be meaningful and the sample complexity to learn the connections would be high. A convolution connection instead of a dense connection helps in alleviating this issue. The convolution operation \((\odot)\) is given by

\[
W[m, n, p] \odot x[m, n, p] = \sum_{i=-h}^{h} \sum_{j=-l}^{l} \sum_{k=-q}^{q} W[i, j, k] \cdot x[m-i, n-j, p-k]
\] (1)

A series of convolutional connections, non-linear activations, and pooling forms a CNN. Subsequently, the voxelized data obtained from the process is fed to the CNN model. The network architecture, shown in Fig. 1\textsuperscript{[1]} comprises of multiple convolution layers with max pooling and dropout layers in-between the convolution layers. Now, we discuss the different non-linear activations used.

(a) Activation function 1: The \texttt{LeakyRelu} activation function was used for the convolution layers in the network, which can be defined as:

\[
\text{LeakyRelu}(x) = \begin{cases} 
1, & x < 0 \\
\alpha x + 1, & x \geq 0 
\end{cases}
\]

where \(\alpha\) is a parameter set by the user. We found that \(\alpha = 0.001\) works the best for the current data and network.

(b) Activation function 2: The \texttt{tanh} function

\[
\text{tanh}(x) = \frac{2}{1 + e^{-2x}} - 1,
\]

was used as the activation function in three dense and fully connected layers close to the output of the network.

Once the CNN has been defined, the weights of each connection may be initialized randomly and then optimized using an appropriate loss function.

(c) Loss function: The loss function used for training:

\[
l = \frac{1}{|\mathcal{D}|} \sum_{k \in \mathcal{D}} (y_{truek} - y_{predk})^2,
\]

where \(\mathcal{D}\) is the dataset to learn from and \(|\mathcal{D}|\) is the number of data points used for training.

With the use of different optimization schemes, we train the CNN and then perform testing accordingly. 

DFT-AIMD Calculations: We utilized ab-initio molecular dynamics (AIMD) simulations as implemented in
Vienna Ab-initio Simulation Package (VASP) for energy, displacements and force calculations for the ternary Ta Nb Mo MEA in a 54-atom supercell. The Perdew-Burke-Ernzerhof (PBE) generalized gradient exchange-correlation potential and the projected-augmented wave (PAW) potentials were used. The 54-atom supercell was generated using SCRAPS methods and was relaxed in the DFT VASP pseudo-potential code with a 400 eV plane-wave energy cutoff and with a Born-Oppenheimer approximation. Each snapshot was performed to check whether a point of interest, e.g., lies inside or outside the corresponding voxel. The test in Eq. 2a was performed to find whether a point of interest lies inside the voxel if the inequalities in Eq. 2a are satisfied.

The DFT-AIMD simulations were performed on Ta Nb Mo 54-atom ternary MEA model in Fig. 2a to extract displacements \( (x, y, z) \) and forces \( (F_x, F_y, F_z) \). A temperature range from 100-1500 K in the steps of every 200 K was considered to include the temperature effect on displacements and forces. The resulting dataset consists of 70k unique snapshots with relevant displacements, forces, and energies of all atoms in Ta Nb Mo 54-atom SCRAP. A structural descriptor \( V \), as expressed in Eq. 3, was employed to capture the interatomic interactions in Ta Nb Mo. The 70k unique snapshots obtained is randomly split into 50k samples for training, 10k samples for validation and 10k samples for testing. This validation strategy enables us to ensure we do not overfit to the training set.

**Voxelization:** Typical DFT-AIMD output is extensive and complex for direct analysis with a deep-convolutional neural network (DNN) because the DFT-AIMD data structure consists of a large set of atomic configurations and properties in a multi-component system. Therefore, we used the idea of voxels to represent atomic configurations. The data in voxel can be represented in a simple cellular structure bounded by a rectangular box, which is analogous to the volume element (V). The voxelization allows to generate a voxel grid with a user-specified resolution. Each voxel in the grid can contain ‘zero’, one or more atoms depending on their spatial \((x,y,z)\) coordinates. The voxel generation also depends on an inside-outside test that compares the atomic coordinates of the atoms with respect to the grid boundaries of the voxel.

The grid-boundary are defined by the minimum and maximum points that can form the diagonal of the volume elements.

We used a voxel based representation of the atomic configuration ternary 54 atom Ta Nb Mo MEAs, with:

\[
0 < \mathbf{k} \cdot \mathbf{u} \leq \mathbf{u} \cdot \mathbf{u} \quad (2a) \\
0 < \mathbf{k} \cdot \mathbf{v} \leq \mathbf{v} \cdot \mathbf{v} \quad (2b) \\
0 < \mathbf{k} \cdot \mathbf{w} \leq \mathbf{w} \cdot \mathbf{w} \quad (2c)
\]

where \( \mathbf{u} = P_x - P_1 \), \( \mathbf{v} = P_y - P_1 \), and \( \mathbf{w} = P_z - P_1 \) are the basis vectors of the voxel and \( \mathbf{k} \) is the scale in atomic locations allows to capture the scale variance on the expense of additional computational time. Additionally, the differences in atom locations are attributed to the effect of kinetic energies in the AIMD simulations at different temperatures by using a proper voxel resolution. A multi-processing approach with NumPy was employed to accelerate the voxelization operations. A first-in-first-out (FIFO) queue is created with each queue package and all 70k snapshots of displacements and force configurations were added to the queue.
**RESULTS AND DISCUSSION**

The effect of voxel resolution and different voxelization methods on the training of the CNN model is an important aspect of testing the proposed framework. To account for the differences in the resolution of the inner-bounding box (ibb) and outer-bounding box (obb), we modify the parameters in Eq. (1) by reducing the filter size and number of filters during the training of ibb and obb. For the obb method, the deep neural-network consists of layers with 256 filters and the kernel size of 2 × 2 × 2 in the first convolution layer. The strides of the convolution filters are 1×1×1 in each convolution layer with a dropout of 0.5 in between the alternate layers. Subsequent layers had a 50% reduction in filters, while kernel size and strides were constant. In ibb model, increasing the filters and their size along with strides had negligible effect on the performance of the model. All the convolution layers have the LeakyReLU activation (α = 0.001) – except the final 3 dense layers, which had a tanh activation. Finally, the entire network is reduced to three fully-connected layers, the layers bearing correspondence to $F_{x,y,z}$ obtained from the DFT-AIMD. For the present implementation, we use the Adam optimizer for minimizing the loss function. The test data was used for validating the performance of the training, while the training and validation was done for 100 epochs. The analysis were carried out in a computing architecture with two Nvidia Tesla V100 GPUs.

In Fig. 4 we have discussed training and validation losses at three resolutions of the voxel grids within ibb. For obb methods. The results in Fig. 4b-d indicates that the obb is more effective than the ibb. For obb in Fig. 4b, training and validation losses are around 0.02 and 0.01, respectively, at the (8×8×8) voxel resolution. Further increase in resolution only marginally improves the performance (validation) for the obb, i.e., the voxel grid for the obb needs to be greater than or equal to 8 in order to minimize the losses. Therefore, we set the voxel resolution to 8×8×8 for obb for optimum performance.

To show the effectiveness of the voxelization framework with respect to a conventional neural network, we plot a comparison of validation losses in Fig. 4a at different resolutions. We found that the CNN with obb method outperformed the fully connected deep neural network representing a dense configuration. However, for the ibb voxelization, the performance was poor in comparison to a full dense configuration, while for the obb methodology shows a significant reduction in the losses, implying an enhanced accuracy. The validation losses for the dense network is around 0.02 while the obb at (16×16×16) voxel
FIG. 4. (a,c) Training and (b,d) validation loss calculated as function of epochs for outer bounding box (obb) and the inner bounding box (ibb). The losses are shown on different voxel resolutions of $4 \times 4 \times 4$, $8 \times 8 \times 8$ and $16 \times 16 \times 16$ for ibb and obb in 54-atom TaNbMo cell. (e) A comparison of validation loss on a dense network against proposed CNN model. Different resolution of voxels were used as an input for ibb ($16 \times 16 \times 16$) and obb ($8 \times 8 \times 8$; $16 \times 16 \times 16$). The inherent nature of the CNN to learn local feature more effectively and perform well even with a higher number of learning parameters can be utilized to develop network architectures to generate the potential energy surface for complex multi-component alloy systems more effectively than the use of traditional dense networks.

The accuracy of the CNN model can be further discussed through a comparison of the DFT-AIMD calculated and CNN-predicted forces in Fig. 5a-i. Figure 5a-f shows the distribution of the 1000 test data points for DFT-AIMD calculated forces ($F_{x,y,z}$) along along ($x,y,z$). The DFT-AIMD calculated $F_{x,y,z}$ (in blue) is largely distributed around the average, i.e., 0, in Fig. 5a-c. We can see the CNN predicted $F_{x,y,z}$ in Fig. 5a-c are in very close agreement with DFT-AIMD forces as shown by the histogram in Fig. 5f and box plot in Fig. 5i. Both DFT-AIMD and CNN datasets show a Gaussian distribution in $F_{x,y,z}$ except for some outliers and correlate very well. The median and the (25, 75)% quantiles match exactly for $F_x$ in Fig. 5b, while $F_y$ and $F_z$ show weak deviations for some data points from the DFT-AIMD forces in Fig. 5c-i. In the case of $F_y$ Fig. 5h, the median of DFT-AIMD and CNN force data are significantly close; however, the width of the box does not completely overlap for the two cases. It shows that the model does not best capture the variance in the DFT-AIMD force data for $F_y$. A similar deviation was found between the DFT-AIMD and CNN $F_z$ data sets in Fig. 5i.

Fig. 5j-l shows a strong positive correlation between the actual (DFT) and predicted (CNN) force values with a Pearson correlation coefficient of 0.942. This further establishes the robustness of the proposed CNN framework. Our framework will provide alternative solutions to the computationally expansive DFT-based simulations by modeling interactions between atoms for designing inter-atomic potential for large-scale calculations. The open-source model and input data are provided online using GitHub (will be provided upon acceptance). More functionality for generating MD-ready potentials will be added in the subsequent stages.

CONCLUSION

In conclusion, we proposed an efficient framework by combining deep-convolution neural networks with voxelization techniques to learn the potential-energy surface of multi-component alloys, including multi-principal-element (random) alloys. Two voxelization strategies: (a) internal bounding box (ibb), and (b) outer bounding box (obb) were used to test the efficacy of the proposed framework. We tested our approach on ternary TaNbMo high-entropy alloy. We show that ibb captures the crisi-
D.B. Miracle and O.N. Senkov, A critical review of high machine-learning (ML) driven frameworks to address the all, the implementation provides pathways for generating atomic potential in multi-principal element alloys. Over-\[
\text{\text{}volutional neural networks (CNNs) for predicting inter-}
\]this is the first approach that uses voxel-based (3D) convolutional neural networks (CNNs) for predicting interatomic potential in multi-principal element alloys. To the best of our knowledge, overall, the implementation provides pathways for generating machine-learning (ML) driven frameworks to address the design of potential-energy surfaces for complex multicomponent alloy systems.

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