

Article

Static Local Lattice Distortion in BCC Refractory High-Entropy Alloys: A DFT Study of NbTaTiV, TiZrNbMo, and HfZrNbMo

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Abstract

Local lattice distortion (LLD) arising from atomic size mismatch is an important structural feature of body-centered cubic (BCC) refractory high-entropy alloys (RHEAs). Reported LLDs are often difficult to compare across alloys because studies use different definitions and reference lattices. In this paper, we computed a consistent static DFT baseline for width-based LLD descriptors for three equimolar quaternary BCC RHEAs: NbTaTiV, TiZrNbMo, and the sparsely reported HfZrNbMo. The alloys were modeled as 128-atom special quasi-random structures and fully relaxed using density functional theory (DFT). Two complementary descriptors were evaluated from the relaxed geometries using a consistently defined reference lattice: a displacement-based metric derived from atomic off-site displacements and a shell-resolved bond length broadening metric for the first and second coordination shells. The resulting LLD descriptors have the lowest values for NbTaTiV, intermediate values for TiZrNbMo, and the highest for HfZrNbMo. Element-resolved analysis shows that individual species contribute differently to the overall distortion, information that is not captured by global descriptors alone. The pretrained MACE machine learning interatomic potential is assessed as a pre-relaxation step prior to DFT relaxation, as well as for screening candidate lattice parameters for HfZrNbMo.

Keywords: high-entropy alloy; NbTaTiV; TiZrNbMo; HfZrNbMo; ab initio calculation; MACE

1. Introduction

Since their introduction [1,2] high-entropy alloys (HEAs) have attracted intensive research interest, and their properties are often discussed in terms of four “core effects” [3]: sluggish diffusion rate, cocktail effect, high configurational entropy, and severe lattice distortion. Initially defined for systems with five or more principal elements [1,2], the HEA concept is now routinely extended to quaternary compositions that retain characteristic disordered solid solution physics of HEAs [4–8]. Here, we use the term in this broader literature sense, while noting that these quaternary systems may also be classified as medium-entropy or multi principal element alloys under stricter definitions. Potential uses of HEA materials include biomedicine [9], electrocatalysis [10], and materials for irradiation-resistant components [11]. Within the wider HEA field, an important subset is formed by refractory high-entropy alloys (RHEAs), which are developed for structural high-temperature applications and are based on high-melting elements such as Nb, Ta, Ti, V, Zr, Mo, and Hf [12–24]. Although prior reviews show that many RHEAs adopt body-centered cubic (BCC) solid solution structures [3,25], the underlying lattice remains



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locally complex as a result of chemical disorder and atomic size mismatch. This disorder at the atomic scale level affects both phase stability and mechanical response and is usually described only indirectly through the composition-based screening descriptors such as valence electron concentration (VEC), atomic size mismatch (δ_r), mixing enthalpy, and electronegativity difference [26–28]. These descriptors are suitable as an initial framework for understanding RHEAs' phase preferences and mechanical stability, but their global, approximate nature means that a greater insight into local environments requires more detailed metrics dependent on structure.

Local lattice distortion (LLD) [29–31] is a structure-resolved descriptor that characterizes static atomic displacements from ideal lattice sites together with the spread of their nearest neighbor distances. LLD is described in the literature in multiple ways depending on the method used, including bond length distributions, width-based local lattice strain descriptors, and statistics of static atomic displacements. Because these measures are defined at different length scales and with different reference states, reported LLD values are often not directly comparable across the literature [29–31]. Recent experimental progress, in particular, total pair distribution function (PDF) analysis of RHEAs [30,31], have demonstrated that LLD in these alloys can be quantified more consistently when determined by distribution widths rather than peak position metrics, in combination with explicit structural modeling. Motivated by this, we frame our LLD analysis in terms of width-based real space descriptors that can be compared directly across alloys. The LLD descriptors reported in this work quantify static disorder extracted from fully relaxed density functional theory (DFT) geometries. LLD results from experimental methods (extended X-ray absorption fine structure (EXAFS), PDF, etc.) [32] are measured at finite temperatures and are therefore affected by a combination of static distortion, thermal motion, and microstructural effects. In this light, our results provide a quantitative static reference baseline for static disorder in an ideal, chemically disordered BCC solid solution. In practice, this baseline can serve as a useful point of comparison for experimentally extracted “static” descriptors, since values that differ substantially from it may reflect differences in thermal treatment, structural modeling, or microstructural state. However, a limitation of global LLD descriptors is that they do not show how distortion is distributed among the constituent elements. As a consequence, similar overall LLD values may arise from different element displacement and local bond length patterns. For this reason, element-resolved LLD (ELLD) is introduced as a complementary analysis that identifies how individual atom species contribute to the total distortion.

Density functional theory models of RHEAs can provide the relaxed atomic coordinates needed to evaluate LLD statistics [30,33], but modeling disordered alloys requires large supercells whose relaxation are computationally expensive [5]. This motivates the development of workflow strategies that lower computational cost without compromising the underlying level of theory. Recent advances in machine learning interatomic potentials (MLIPs) [34,35] make it practical to use MLIP-based first stage relaxation prior to DFT optimization, and as a result, reducing the overall relaxation cost.

The work presented in this paper studies three equimolar quaternary BCC RHEAs: NbTaTiV, TiZrNbMo, and HfZrNbMo. The alloys are chosen to span increasing atomic size mismatch parameter (δ_r) within a closely related BCC RHEA design space. Using a consistent workflow across this series, with increasing δ_r , enables a focused comparison of LLD. In addition, equation of state (EOS) curves are computed to obtain the bulk modulus for all three alloys, as well as density of state (DOS) curves to provide a supporting context for DFT results. In this work, the pretrained MACE MLIP [36] is employed as a pre-relaxation step and lattice parameter screening tool. The method's robustness is assessed

by comparing the final DFT-relaxed energies and geometries obtained from direct DFT relaxations with those obtained by pre-relaxing with MACE, followed by DFT relaxation.

Within this investigation, NbTaTiV is used as a benchmark alloy with both experimental and DFT data reported in the literature [5] while for equimolar TiZrNbMo [37] BCC DFT work and experimental results exist on near-equiatomic and related Ti-Zr-Nb-Mo alloys. In contrast, data published specifically on equimolar HfZrNbMo remain comparatively scarce. Related alloys of higher order that contain the Hf-Zr-Nb-Mo subset have been studied, such as experimental studies of the mechanical properties of the MoNbHfZrTi [38,39] and HfMoNbTaZr [20]. To the best of our knowledge, a consistent DFT from a special quasi-random structure (SQS) baseline for distribution-based static LLD descriptors for the equimolar BCC quaternary HfZrNbMo has not been systematically reported. This motivates the present work, in which we report the DFT-relaxed structure and LLD statistics for equimolar HfZrNbMo using the same protocol applied to NbTaTiV and TiZrNbMo. We also show that MLIP pre-relaxation can lower the computational cost of large supercell DFT RHEA optimization.

2. Computational Modeling and Methods

2.1. Structure Models and Workflow

Three equimolar BCC RHEAs (NbTaTiV, TiZrNbMo, HfZrNbMo) were selected based on composition-based screening descriptors (Table 1), with increasing both atomic size mismatch parameter (δ_r) and electronegativity difference ($\Delta\chi$) while other descriptors (VEC = 4.75 [40] and configurational entropy [26] $\Delta S_{\text{mix}} = 1.386 R$, where R is the gas constant) are constant. Atomic size mismatch is calculated using $\delta_r(\%) = 100 \sqrt{\sum_i c_i (1 - r_i/\bar{r})^2}$ (where $\bar{r} = \sum_i c_i r_i$, and concentration is $c_i = 0.25$) [26], electronegativity difference using $\Delta\chi = \sqrt{\sum_i c_i (\chi_i - \bar{\chi})^2}$ (where $\bar{\chi} = \sum_i c_i \chi_i$) [27]. Metallic radii for Nb, Ta, Ti, V, Zr, and Hf were taken from Vlasák et al. [41] and are $r_{\text{Nb}} = r_{\text{Ta}} = r_{\text{Ti}} = 1.43 \text{ \AA}$, $r_{\text{V}} = 1.31 \text{ \AA}$, $r_{\text{Zr}} = r_{\text{Hf}} = 1.56 \text{ \AA}$. The metallic radius of Mo is obtained from [27] and is $r_{\text{Mo}} = 1.363 \text{ \AA}$. The Pauling electronegativity for each element is $\chi_{\text{Nb}} = 1.6$, $\chi_{\text{Ta}} = 1.5$, $\chi_{\text{Ti}} = 1.54$, $\chi_{\text{V}} = 1.63$, $\chi_{\text{Zr}} = 1.33$, $\chi_{\text{Hf}} = 1.3$, and $\chi_{\text{Mo}} = 2.16$ [27].

Table 1. Composition-based screening descriptors for the three equimolar BCC RHEAs (NbTaTiV, TiZrNbMo, and HfZrNbMo): atomic size mismatch parameter (δ_r (%)) and electronegativity difference ($\Delta\chi$ (Pauling scale)).

Alloy	δ_r (%)	$\Delta\chi$
NbTaTiV	3.71	0.051
TiZrNbMo	4.94	0.307
HfZrNbMo	5.76	0.345

All RHEA configurations discussed in this paper were modeled by special quasi-random structures (SQSs) generated using the Monte Carlo SQS (MCSQS) module of ATAT [42–44] (via NanoHub). In the main analysis, one 128-atom SQS was used for each alloy. The initial lattice parameters (a_0) of 128-atom BCC SQS supercells are chosen using the best available data following standard practice in HEA computational literature. In the case of NbTaTiV, a_0 is taken from prior literature report for equimolar BCC NbTaTiV to be $3.24 \text{ \AA}$, while for TiZrNbMo a_0 was chosen based on the reported BCC lattice constants. For HfZrNbMo, the lattice constant is taken to be $3.38 \text{ \AA}$ based on the method described in Section 2.3.

2.2. DFT Setup

DFT calculations were performed using GPAW (25.7.1b1) [45,46] in ASE (3.26.0) [47] in plane-wave mode with the Perdew–Burke–Ernzerhof (PBE) exchange–correlation functional. A kinetic energy cutoff was set to 450 eV while Fermi–Dirac smearing was set to 0.10 eV. Geometry optimization was performed, relaxing both atomic and cell coordinates using the UnitCell filter and the Broyden–Fletcher–Goldfarb–Shanno (BFGS) optimizer (maximum ionic step set to 0.04 up to 300 steps). Two distinct k-point settings were utilized. Γ -point only relaxations served as the reference endpoint in the MACE assessment (Section 2.3), with a target force threshold of 0.02 eV/Å. All postprocessing quantities (LLD, ELLD, DOS, and EOS) reported in this work were calculated from structures relaxed using a Γ -centered $2 \times 2 \times 2$ Monkhorst–Pack k-point mesh, with a target force threshold of 0.04 eV/Å.

2.3. MACE

To evaluate the effectiveness of MLIP-assisted DFT workflows for HEA structure relaxation, a computational benchmark was performed comparing two pathways: MLIP pre-relaxation followed by DFT refinement versus direct DFT relaxation. Both pathways were initiated from identical SQS starting geometries. In the first pathway, the SQS starting structure is pre-relaxed with the pretrained MACE-MP-0 (mace-torch v0.3.14, large model) [36,48]. Variable cell optimization used UnitCellFilter with the limited-memory BFGS (L-BFGS) optimizer with a target force threshold of 0.05 eV/Å. The resulting geometry is then used as a starting point for GPAW relaxation. In the second pathway, only GPAW optimization is performed. Both pathways follow the same DFT protocol for relaxation in the Γ -point described in Section 2.2.

To the best of our knowledge, a BCC lattice parameter for equimolar HfZrNbMo has not been reported in prior experimental or computational work. Guided by the data for closely related refractory BCC alloys [49], the starting lattice parameter was selected using MACE for isotropic lattice relaxation. It was scanned over lattice parameter values (3.36 Å–3.40 Å) with a 0.01 Å step, fitted with a third-order Birch–Murnaghan equation in the search for the one with the lowest energy.

2.4. LLD

To quantify static LLD from the DFT-relaxed structures in a reproducible way, we employ width-based lattice strain descriptors [30,31]. Two complementary distribution-based descriptors are used: (i) a metric based on atomic off-site displacement from ideal lattice positions, and (ii) the width of nearest neighbor bond length distributions evaluated within reference labeled 1NN and 2NN coordination shells. This approach follows prior work on chemically complex alloys, emphasizing explicit metric definitions and robust reference structure and neighboring shell labeling [29–31]. The unrelaxed 128-atom BCC SQS supercell serves as the reference configuration with the same atomic ordering of species as the final configuration. To avoid treating uniform changes in the cell volume and shape as LLD, reference configuration fractional coordinates ($\mathbf{s}_i^{\text{ref}}$) were mapped into the relaxed supercell matrix ($\mathbf{H}^{\text{rel}}$) to determine atomic reference positions ($\mathbf{r}_i^{\text{site}}$) in the final geometry:

$$\mathbf{r}_i^{\text{site}} = \mathbf{H}^{\text{rel}} \mathbf{s}_i^{\text{ref}}. \quad (1)$$

Defined this way, LLD reflects only local, non-affine atomic displacements relative to the embedded reference sites.

Atomic displacements were defined using the minimum image convention (MIC) under periodic boundary conditions between each relaxed atom position and its embedded reference site:

$$\Delta \mathbf{r}_i = \text{MIC}(\mathbf{r}_i^{\text{rel}} - \mathbf{r}_i^{\text{site}}). \quad (2)$$

The final atomic displacement vector ($\mathbf{u}_i$) of the specific site i is obtained by removing residual rigid translation by applying a zero-mean gauge:

$$\mathbf{u}_i = \Delta \mathbf{r}_i - \langle \Delta \mathbf{r} \rangle. \quad (3)$$

The displacement-based LLD ($\sigma_{s,u}$) width is then defined following Hu et al. [30] as the isotropic 1D root mean square width of the distribution of atomic displacement vectors $\mathbf{u}_i$ as:

$$\sigma_{s,u} = \left(\sqrt{\frac{\langle |\mathbf{u}|^2 \rangle}{3}} \right). \quad (4)$$

The LLD descriptor based on displacement ($\varepsilon_{s,u}$) comparable between different RHEAs is defined by normalizing $\sigma_{s,u}$ by the BCC hard-sphere reference radius $\bar{r} = (\sqrt{3}/4)a_{\text{eff}}$ (where $a_{\text{eff}} = (2V/N)^{1/3}$ is obtained from the relaxed supercell volume V and atom count, N):

$$\varepsilon_{s,u} = 100 \frac{\sigma_{s,u}}{\bar{r}}. \quad (5)$$

The second LLD descriptor, the shell-resolved bond length strain, $\varepsilon_{s,l}^{(n)}$, is defined to quantify bond length disorder within a specific coordination shell (n). Here we evaluate the first two coordination shells, $n \in \{1\text{NN}, 2\text{NN}\}$. For each atomic reference site (i) in the embedded reference BCC lattice, there are eight first shell nearest neighbors (1NNs) and six second shell nearest neighbors (2NNs).

After DFT relaxation, we compute the relaxed bond lengths from minimum image separation vectors under periodic boundary conditions:

$$d_{ij}^{(n)} = \left| \text{MIC}(\mathbf{r}_j^{\text{rel}} - \mathbf{r}_i^{\text{rel}}) \right|, (i, j) \in n. \quad (6)$$

The bond length specific for certain shell distribution is defined with a set $\{d_{ij}^{(n)}\}$ with the mean $\mu^{(n)} = \langle d^{(n)} \rangle$ and standard deviation $\sigma^{(n)} = \text{std}(d^{(n)})$. Dimensionless shell-resolved bond length strain is now defined as:

$$\varepsilon_{s,l}^{(n)} = \frac{\sigma^{(n)}}{\mu^{(n)}}. \quad (7)$$

The necessary consistency in neighbor labeling is ensured by defining 1NN/2NN neighbor lists from the embedded ideal lattice positions. After relaxation, we verified that neighboring atoms did not swap sites.

To better understand the role of each element in the LLD, we also report element-resolved LLD (ELLD). This is done by grouping the distributions by atomic species: the distributions of normalized displacement magnitudes ($|\mathbf{u}|/\bar{r}$), and element-centered first neighbor deviations ($\Delta r_{1\text{NN}}(i \rightarrow j)$). For each central atom i , we define the element-centered first neighbor deviation as $\Delta r_{1\text{NN}}(i) = d_{ij}^{(1\text{NN})} - d_{1\text{NN}}^{\text{ideal}}$, computed over all 1NN bonds (i, j). Here $d_{ij}^{(1\text{NN})}$ is the relaxed 1NN bond length (Equation (6)), and $d_{1\text{NN}}^{\text{ideal}} = (\sqrt{3}/2)a_{\text{eff}}$ is the ideal BCC 1NN distance associated with the a_{eff} of the relaxed cell used throughout the LLD normalization (Equation (5)). The $\Delta r_{1\text{NN}}$ is reported in Å and grouped by the central element.

2.5. The Equation of State and Electronic Density of State

The equation of state (EOS) analysis in this paper provides a systematic method for comparing equilibrium volumes and small strain compressibility across alloys, while elastic constants and full mechanical property studies are outside the scope of this research. EOS curves were constructed from DFT total energies computed at isotropically scaled volumes. Starting from the reference supercell volume V_{ref} , uniform scaling factor s is applied such that $V = V_{ref}s^3$ using $s = \{0.985, 0.990, 0.995, 1.000, 1.005, 1.010, 1.015\}$. The resulting $E(V)$ data were fitted to the third-order Birch–Murnaghan form [50]:

$$E(V) = E_0 + \frac{9V_0B_0}{16} \left\{ \left[\left(\frac{V_0}{V} \right)^{\frac{2}{3}} - 1 \right]^3 B'_0 + \left[\left(\frac{V_0}{V} \right)^{\frac{2}{3}} - 1 \right]^2 \left[6 - 4 \left(\frac{V_0}{V} \right)^{\frac{2}{3}} \right] \right\}, \quad (8)$$

to determine the equilibrium volume V_0 , effective BCC lattice parameter a_{EOS} , and bulk modulus B_0 .

The electronic density of state (DOS) is calculated using the ASE DOS module applied to the final DFT results. The DOS was evaluated with 0.2 eV Gaussian broadening, and a Γ -centered $2 \times 2 \times 2$ k-point mesh. The DOS was included as a supporting context for DFT analysis and is therefore presented only in Appendix A.

3. Results and Discussion

Our three configurations, NbTaTiV, TiZrNbMo, and HfZrNbMo, were modeled by special quasi-random structures generated using the Monte Carlo SQS module of ATAT. Figure 1 schematically shows the initial 128-atom BCC SQS atom placement of Nb, Ta, Ti, V, Zr, Mo, and Hf from the three alloys, as visualized using VESTA [51].

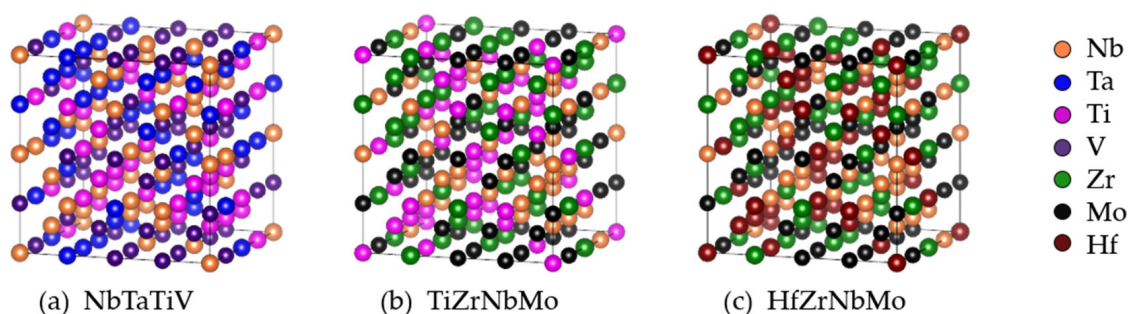


Figure 1. Representative initial 128-atom BCC SQS atomic structures of (a) NbTaTiV, (b) TiZrNbMo, and (c) HfZrNbMo sorted by element color.

3.1. Density Functional Theory Optimization

According to our previously described DFT protocol, the initial 128-atom BCC SQS models for three alloys all converged to stable BCC-like geometries. The lattice parameter for NbTaTiV is consistent with earlier large-cell DFT studies that report a BCC lattice parameter of approximately 3.22 Å [52] for equimolar NbTaTiV, supporting the reliability of the present 128-atom GPAW setup. The effective BCC lattice parameter for our three alloys obtained from DFT are for NbTaTiV 3.23 Å, for TiZrNbMo 3.31 Å, and for HfZrNbMo 3.39 Å, reflecting the increasing average metallic radius and atomic size mismatch. All LLD/ELLD, EOS, and DOS results are computed from the structures relaxed in DFT in a $2 \times 2 \times 2$ k-mesh. For LLD/ELLD, the reference lattice is defined by embedding the fractional coordinates of the unrelaxed 128-atom BCC SQS into the relaxed cell (Section 2.4).

The reference structure for each alloy is fully converged DFT with convergence parameters detailed in Methods. Static single-point energy calculations were performed at isotropically scaled volumes. The resulting equation of state data presented in the Figure 2

are the resulting points for (a) NbTaTiV, (b) TiZrNbMo, and (c) HfZrNbMo, which were fitted to a third-order Birch–Murnaghan equation (Equation (8)) to determine the equilibrium volume (V_0), equilibrium BCC lattice parameter (a_{EOS}), and bulk modulus (B_0). The fits yield a_{EOS} values of 3.23 Å, 3.32 Å, and 3.39 Å as well as per atom volumes of 16.83 Å³, 18.25 Å³, and 19.48 Å³ for NbTaTiV, TiZrNbMo, and HfZrNbMo, respectively, with corresponding bulk moduli of 160.9 GPa, 146.1 GPa, and 141.6 GPa. The extracted bulk moduli primarily serve as a consistency check that the relaxed cell lies near the true energy minimum. For all three alloys, the chosen initial lattice constants match the volume values in the vicinity of energy minima (Figure 2).

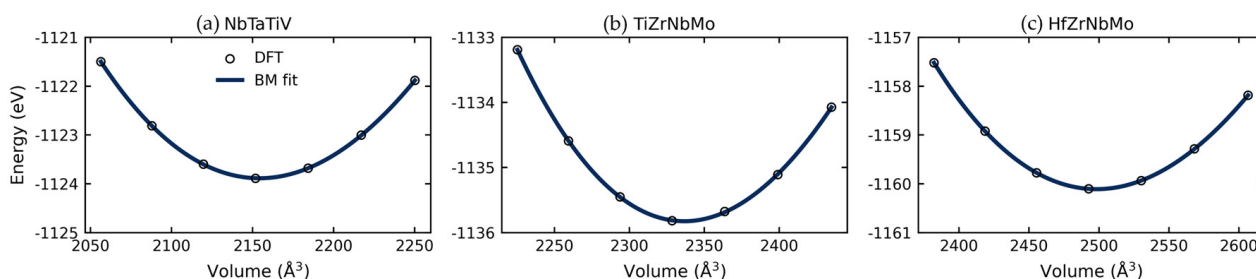


Figure 2. Equation of state curves for BCC (a) NbTaTiV, (b) TiZrNbMo, and (c) HfZrNbMo obtained from isotropic volume scaling of 128-atom disordered supercells. Solid lines are third-order Birch–Murnaghan fits.

3.2. MACE-Assisted Workflow

For HfZrNbMo, the MACE-guided lattice parameter screening described in Methods yielded a starting value close to the final DFT-relaxed effective lattice parameter, confirming its practical usefulness for initializing the subsequent DFT relaxation. In each of the three compositions studied, DFT relaxation at the Γ -point for both pathways (MACE pre-relaxed and initial SQS structures) yielded equivalent final states, with total energies differing by less than 0.6 meV/atom. Lattice parameters and cell shapes were indistinguishable between pathways. MACE pre-relaxation reduced DFT wall time by approximately 20%. Given the preserved DFT endpoint and reduced computational time, MACE can accelerate the computation of large supercell DFT relaxations.

3.3. Local Lattice Distortion

We quantify static LLD in DFT-relaxed 128-atom BCC SQS supercells in Figure 3 for NbTaTiV (blue), TiZrNbMo (orange), and HfZrNbMo (green) using two width-based descriptors: the displacement metric $\epsilon_{s,u}$, and shell-resolved bond length metric $\epsilon_{s,l}^{(n)}$. The distribution of normalized displacement magnitudes $|\mathbf{u}|/\bar{r}$ is plotted in Figure 3a (dashed lines), as well as the kernel density estimate (KDE) (solid lines). The histogram provides a dimensionless view of static off-site displacements that indicates whether differences arise among the studied alloys from a uniform broadening or from more weight at a larger $|\mathbf{u}|/\bar{r}$. Figure 3b compares LLD, $\epsilon_{s,u}$, across all three alloys. HfZrNbMo shows the broadest $|\mathbf{u}|/\bar{r}$ and the largest $\epsilon_{s,u}$ among the studied systems.

Figure 4 presents the normalized bond length distribution for reference labeled 1NN (blue lines) and 2NN (orange lines) coordination shells of (a) NbTaTiV, (b) TiZrNbMo, and (c) HfZrNbMo, plotted as $d^{(n)}/\mu^{(n)}$ for visualization purposes. The corresponding shell broadening is quantified with $\epsilon_{s,l}^{(n)}$ in Table 2. In the case of HfZrNbMo, the broadest distribution is present in both shells (Figure 4c), consistent with the largest value of the $\epsilon_{s,l}^{(n)}$ descriptor in Table 2. By contrast, Figure 4a,b shows the narrowest bond length distribution for NbTaTiV, and as an intermediate one lies TiZrNbMo. Across all three alloys in Figure 4

can be seen that 2NN distribution width is broader than 1NN, indicating that the bond length broadening extends into the second coordination shell.

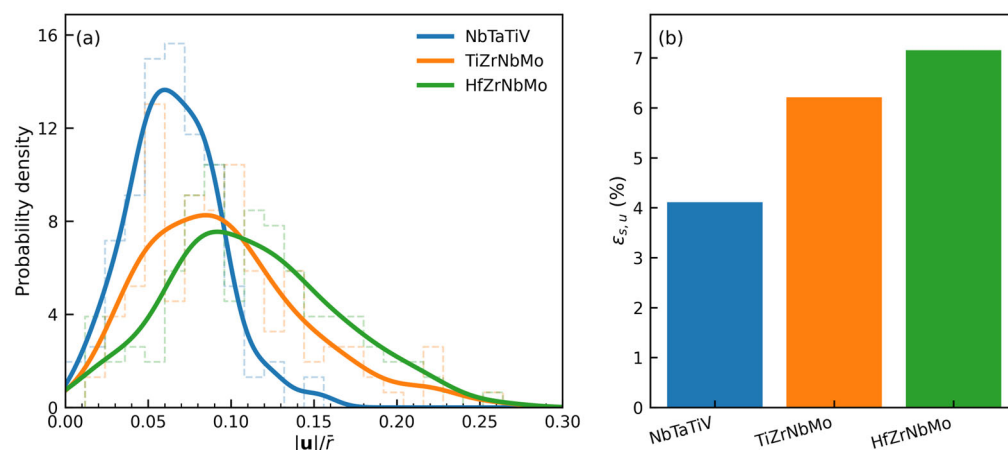


Figure 3. Displacement-based LLD in DFT-relaxed 128-atom BCC SQS for NbTaTiV (blue), TiZrNbMo (orange), and HfZrNbMo (green): (a) probability density of the normalized off-site displacement magnitude $|u|/\bar{r}$ (solid lines: KDE, dashed lines: normalized histogram), (b) corresponding displacement-width descriptor $\varepsilon_{s,u} = 100\sigma_{s,u}/\bar{r}$.

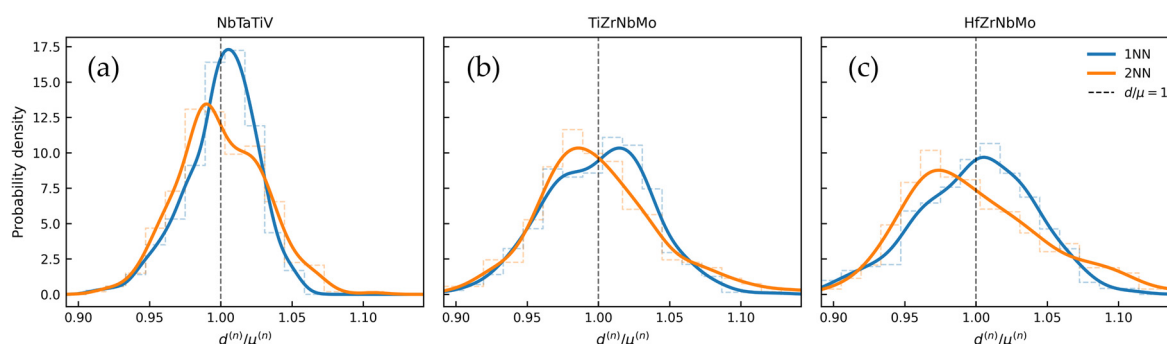


Figure 4. Shell-resolved bond length broadening in DFT-relaxed 128-atom BCC SQS. Probability density of normalized distances $d^{(n)}/\mu^{(n)}$ for the 1NN (blue) and 2NN (orange) shells in (a) NbTaTiV, (b) TiZrNbMo, and (c) HfZrNbMo. Solid lines show a kernel density estimate (KDE), i.e., a smoothed estimate of the probability density; and dashed outlines show normalized histograms. Dashed vertical lines mark the corresponding ideal shell reference positions.

Table 2. Summary of static local lattice distortion (LLD) descriptors for DFT-relaxed 128-atom BCC SQS supercells. The displacement metric, $\varepsilon_{s,u}$, and shell-resolved bond length broadening $\varepsilon_{s,l}$ (1NN) and $\varepsilon_{s,l}$ (2NN) are reported in percentages, where a_{eff} is the effective BCC lattice parameter derived from the relaxed cell volume.

Alloy	a_{eff} (Å)	$\varepsilon_{s,u}$ (%)	$\varepsilon_{s,l}(1NN)$ (%)	$\varepsilon_{s,l}(2NN)$ (%)
NbTaTiV	3.227	4.11	2.48	3.01
TiZrNbMo	3.313	6.21	3.68	4.24
HfZrNbMo	3.387	7.15	4.04	4.89

Table 2 summarizes the LLD descriptors derived from Figures 3 and 4 for all three alloys. Both the displacement-based metric $\varepsilon_{s,u}$ and the shell-resolved bond length metrics $\varepsilon_{s,l}(1NN)$ and $\varepsilon_{s,l}(2NN)$ are lowest for NbTaTiV, intermediate for TiZrNbMo and the highest for HfZrNbMo. Specifically, $\varepsilon_{s,u}$ is 4.11% for NbTaTiV, 6.21% for TiZrNbMo and 7.15% for HfZrNbMo, corresponding to relative increases of about 50% and 74% with respect to NbTaTiV. Additional NbTaTiV SQS realizations were examined as a sensitivity

check and they did not change the conclusion that NbTaTiV shows the smallest distortion among the three alloys. The bond length broadening shows a similar progression: $\varepsilon_{s,l}(1\text{NN})$ increases from 2.48% to 3.68% and 4.04%, while $\varepsilon_{s,l}(2\text{NN})$ increases from 3.01% to 4.24% and 4.89%, so that the alloy with the largest LLD descriptors (HfZrNbMo) exhibits a roughly 60–65% larger shell-resolved bond length strain than NbTaTiV. This LLD descriptor ordering is consistent with composition-based screening descriptors in Table 1. This compositional ordering is also qualitatively consistent with the recent literature [53], which reported especially severe local lattice distortion in BCC refractory alloys containing Zr and/or Hf. Within the present DFT/SQS protocol, the larger distortion obtained for TiZrNbMo and especially HfZrNbMo therefore follows the same overall trend. In the present research, Zr and Hf are the largest constituent species, so their presence increases the size contrast within the BCC lattice. A reasonable structural interpretation is that this promotes less uniform accommodation of interatomic distances than in NbTaTiV, with the effect expected to be most pronounced in HfZrNbMo, where two large Group IV elements coexist with the comparatively smaller Mo species. A more detailed element-resolved discussion of this behavior is given below.

Our static DFT LLD descriptors provide a static reference based on geometry for the scale of local broadening in these alloys. In finite temperature total scattering analysis (PDF, EXAFS, etc.), peak widths generally reflect both static disorder and thermal motion. Separating these contributions is nontrivial and depends on the model in use [30]. In this context, our static values can serve as a reference point for the expected magnitude of the static component. For NbTaTiV, our displacement-based $\varepsilon_{s,u}$ is smaller than the “static” lattice strain reported by Hu et al. [30] from Rietveld/PDF analysis. A difference in magnitude is expected because the experimental “static” term is obtained via model-dependent deconvolution of finite temperature data, whereas our values come from static DFT-relaxed geometries. For TiZrNbMo and HfZrNbMo, we did not find directly comparable experimental LLD values at the time of writing. HfZrNbMo in particular remains sparsely reported, so these results may be useful as a reference for future work.

The global LLD descriptors above are useful for comparing different alloys, but they do not show how the distortion is distributed across elements. We address this by calculating element-resolved LLD (ELLD) descriptors, presented in the next figures.

In Figure 5, the element-resolved distributions of normalized displacement magnitudes $|\mathbf{u}_i|/\bar{r}$ for DFT-relaxed 128-atom BCC SQS of (a) NbTaTiV, (b) TiZrNbMo, and (c) HfZrNbMo are shown and colored by element (Nb-blue, Ta-orange, Ti-green, V-red, Zr-brown, Mo-purple, and Hf-pink). Box and swarm plots represent distributions grouped by element, where each element has 32 atoms.

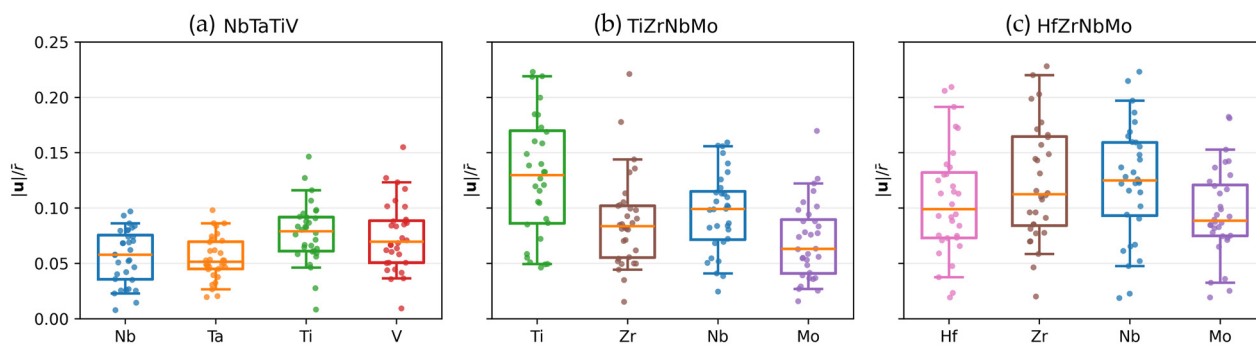


Figure 5. Element-resolved normalized displacement magnitudes $|\mathbf{u}_i|/\bar{r}$ for DFT-relaxed 128-atom BCC SQS of (a) NbTaTiV, (b) TiZrNbMo, and (c) HfZrNbMo. Box and swarm plots represent distributions grouped and colored by element (Nb-blue, Ta-orange, Ti-green, V-red, Zr-brown, Mo-purple, and Hf-pink).

In Figure 6, the element-centered first neighbor bond length deviations for DFT-relaxed 128-atom BCC SQS of (a) NbTaTiV, (b) TiZrNbMo, and (c) HfZrNbMo are shown and colored by central element (Nb-blue, Ta-orange, Ti-green, V-red, Zr-brown, Mo-purple, and Hf-pink). Box plots are grouped by central species (256 bonds per element); the horizontal zero line marks the ideal BCC 1NN distance.

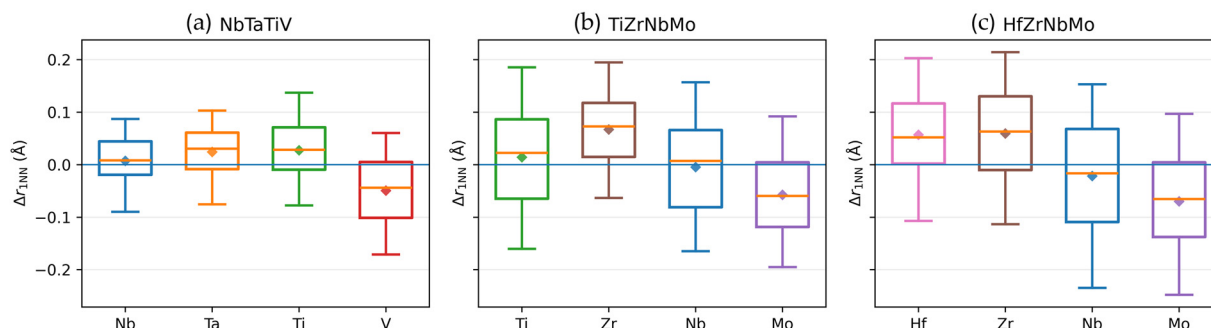


Figure 6. Element-centered first neighbor bond length deviations in DFT-relaxed 128-atom BCC SQS of (a) NbTaTiV, (b) TiZrNbMo, and (c) HfZrNbMo. Box plots are grouped by central species (256 bonds per element); the horizontal zero line marks the ideal BCC 1NN distance. The ideal BCC 1NN distance is $d_{1NN}^{ideal} = \left(\sqrt{3}/2\right)a_{eff}$, with a_{eff} taken from the relaxed cell volume (Equation (5)).

Element-resolved LLD shows how the distortion is distributed across elements. Two alloys with similar $\varepsilon_{s,u}$ can exhibit completely different trends when it comes to the local accommodation of distortion. The character of that distortion, and whether it appears as off-site atomic displacement or as systematic 1NN contraction and expansion, is equally invisible to a global metric. Consistent with the global $\varepsilon_{s,u}$ values, the overall spread of the ELLD displacement distributions follows the same least-to-most distorted ordering, while ELLD reveals how that broadening is partitioned among elements. For NbTaTiV, it is noticeable from Figure 5a that Nb and Ta show the lowest typical displacements, while Ti and V are shifted to larger values (higher medians and broader spreads). In Figure 6a, V shows a negative median bond length deviation in its neighborhood, where relatively large displacements are paired with 1NN contraction. Here it should be highlighted that a large $|\mathbf{u}_i|$ does not necessarily correspond to 1NN expansion. This indicates that the distortion is not captured by a uniform radial bond stretch alone. In TiZrNbMo, the ELLD in both Figures 5b and 6b depends much more on the specific element. Ti exhibits the largest median and the widest spread (including an upper tail), whereas Mo has the smallest typical displacements, and Nb and Zr are intermediate. The element-centered first neighbor bond length distributions in Figure 6b add the missing microscopic interpretation: Zr is clearly positive (locally longer 1NN distances), Mo is negative (locally shorter 1NN distances), while Ti sits near zero to slightly positive, and Nb is near zero with a broad spread. Overall, Ti carries the displacement amplitude, Zr expands, and Mo contracts. This element-by-element partitioning is not accessible when $\varepsilon_{s,u}$ and $\varepsilon_{s,l}$ (1NN) are reported only as global values. In the HfZrNbMo, the $|\mathbf{u}_i|/\bar{r}$ distributions are broadly elevated across elements: Nb has the highest typical $|\mathbf{u}_i|/\bar{r}$ and Mo the lowest. The more uniform distribution of ELLD across elements in HfZrNbMo, relative to the more element-differentiated patterns in TiZrNbMo, may reflect the fact that three of the four constituents (Hf, Zr, and Nb) have relatively similar metallic radii, leaving Mo as the primary outlier in terms of atomic size. This element-resolved partitioning supports the interpretation that the stronger distortion in the alloys that contain Zr and/or Hf arises from heterogeneous local accommodation of neighbor distances, rather than from atomic size mismatch alone. In particular, the 1NN bond length distributions show that locally expanded and contracted environments coexist and are distributed differently across species, rather than reflecting a uniform bond

expansion. This helps explain why the alloys containing Zr/Hf exhibit larger global LLD values within the present alloy set. The analysis here remains structural in scope and does not by itself establish the underlying electronic mechanism.

To make MACE–DFT differentiation more explicit, Appendix B includes additional figures parallel to Figures 5 and 6, enabling comparison of the element-resolved LLD results from only MACE-relaxed structures with the corresponding DFT results. Across all three alloys, the similar overall qualitative behavior is preserved, although some quantitative differences appear in the detailed distributions, supporting the use of MACE as an efficient first stage relaxation method, while the final DFT-relaxed structures must remain the basis for the main analysis.

4. Conclusions

Three equimolar quaternary BCC RHEAs (NbTaTiV, TiZrNbMo, and the sparsely reported HfZrNbMo) were modeled as 128-atom SQS supercells and fully relaxed with static DFT, followed by postprocessing of static local lattice width-based distortion metrics (LLD), equation of state (EOS), and density of state (DOS). We quantified LLD and ELLD from the relaxed geometries relative to embedded reference sites defined by the unrelaxed SQS fractional coordinates mapped into the relaxed cell. Among the three alloys studied, the LLD descriptors are smallest for NbTaTiV, intermediate for TiZrNbMo, and largest for HfZrNbMo, which is in accordance with simple composition-based screening descriptors. This trend is consistent with the stronger distortion expected in the Zr/Hf-containing alloys, where larger local size and chemistry contrast lead to less uniform local accommodation of neighbor distances. The 2NN distributions are broader than the 1NN distributions, indicating that bond length broadening extends beyond the first coordination shell within this DFT/SQS protocol. ELLD has shown that similar global LLD magnitudes can arise from different microscopic distortion patterns.

The use of MACE MLIP in RHEAs workflows was investigated. For all three alloys, MACE was used as a pre-relaxation step, reducing the DFT computation time by 20%. Subsequent DFT relaxation of both MACE pre-relaxed and initial structures yielded equivalent results. Also, it is shown that in the case of HfZrNbMo, MACE can be used for efficiently screening the initial lattice constant prior to final DFT relaxation.

Future work could extend this analysis to additional BCC RHEA compositions and to comparisons with experimental or simulation distortion measures.

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Abbreviations

The following abbreviations are used in this manuscript:

BCC	Body-centered cubic
BFGS	Broyden–Fletcher–Goldfarb–Shanno
DFT	Density functional theory
DOS	Density of state
EOS	Equation of state
EXAFS	Extended X-ray absorption fine structure
HEA	High-entropy alloys
KDE	Kernel density estimate
L-BFGS	Limited-memory BFGS
LLD	Local lattice distortion
MCSQS	Monte Carlo special quasi-random structure
MIC	Minimum-image convention
MLIP	Machine learning interatomic potentials
PBE	Perdew–Burke–Ernzerhof
PDF	Pair distribution function
RHEA	Refractory high-entropy alloys
SQS	Special quasi-random structure
TDOS	Total DOS
VEC	Valence electron concentration

Appendix A

Total DOS (TDOS) was computed around the Fermi level (E_F) to provide a supporting context for the DFT results of the three DFT-relaxed 128-atom BCC SQS RHEAs. In Figure A1 the TDOS of NbTaTiV (blue line), TiZrNbMo (orange line), and HfZrNbMo (green line) normalized per atom and referenced to the E_F are shown. For all three alloys, a finite TDOS is present at E_F (dashed line), confirming their metallic electronic character [54]. Our NbTaTiV DOS aligns well with the literature one [5].

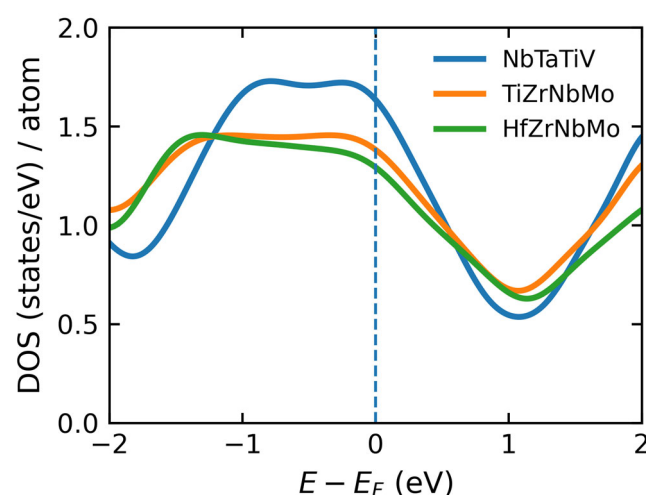


Figure A1. Total density of states for DFT-relaxed 128-atom BCC SQS of NbTaTiV (blue line), TiZrNbMo (orange line), and HfZrNbMo (green line) normalized per atom. Energies are referenced to the Fermi level (dashed line).

Appendix B

In Figure A2 the element-resolved distributions of normalized displacement magnitudes $|\mathbf{u}_i|/\bar{r}$ for 128-atom BCC SQS relaxed using MACE only of (a) NbTaTiV, (b) TiZrNbMo, and (c) HfZrNbMo are shown and colored by element (Nb-blue, Ta-orange, Ti-green, V-red,

Zr-brown, Mo-purple, and Hf-pink). Box and swarm plots represent distributions grouped by element, where each element has 32 atoms. Figure A3 presents the element-centered first neighbor bond length deviations for MACE-relaxed 128-atom BCC SQS of (a) NbTaTiV, (b) TiZrNbMo, and (c) HfZrNbMo and is colored by the central element (Nb-blue, Ta-orange, Ti-green, V-red, Zr-brown, Mo-purple, and Hf-pink). Box plots are grouped by central species (256 bonds per element); the horizontal zero line marks the ideal BCC 1NN distance. Comparing with Figures 5 and 6, the same broad qualitative picture is retained across all three alloys, while quantitative differences are visible in the detailed distributions. This supports the use of MACE as a practical first stage relaxation tool, whereas the final DFT-relaxed structures cannot be replaced in the main analysis.

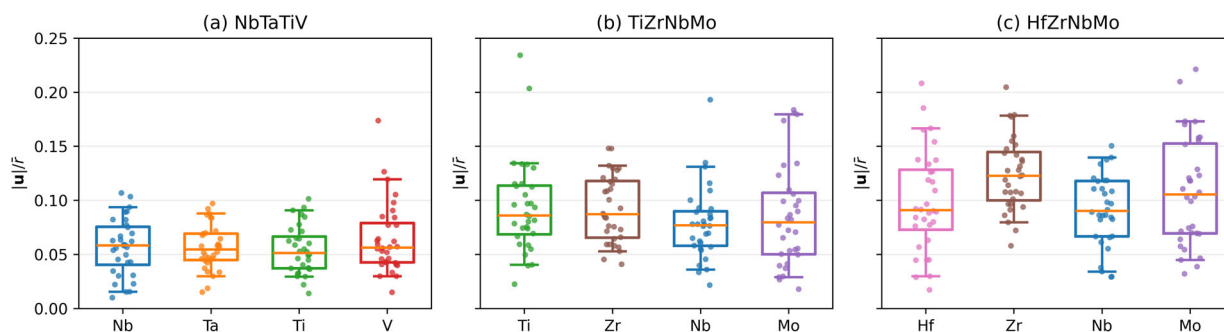


Figure A2. Element-resolved normalized displacement magnitudes $|u_i|/\bar{r}$ for MACE-relaxed 128-atom BCC SQS of (a) NbTaTiV, (b) TiZrNbMo, and (c) HfZrNbMo. Box and swarm plots represent distributions grouped and colored by element (Nb-blue, Ta-orange, Ti-green, V-red, Zr-brown, Mo-purple, and Hf-pink).

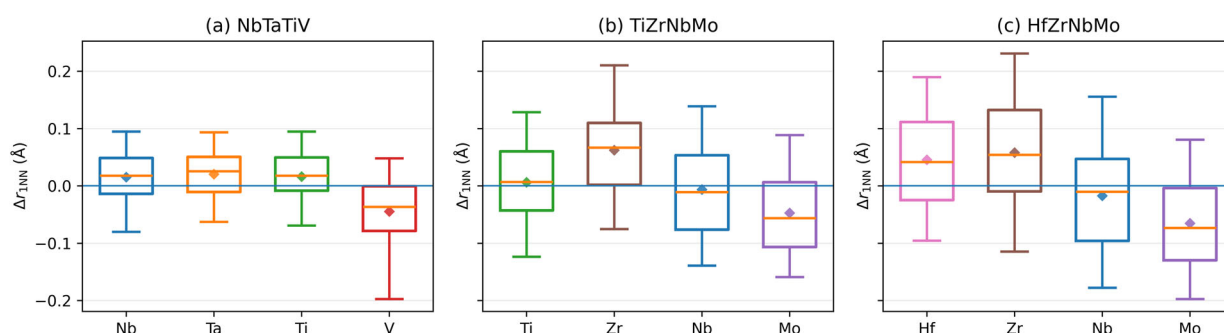


Figure A3. Element-centered first neighbor bond length deviations in MACE-relaxed 128-atom BCC SQS of (a) NbTaTiV, (b) TiZrNbMo, and (c) HfZrNbMo. Box plots are grouped by central species (256 bonds per element); the horizontal zero line marks the ideal BCC 1NN distance. The ideal BCC 1NN distance is $d_{1NN}^{ideal} = \left(\sqrt{3}/2\right)a_{eff}$, with a_{eff} taken from the relaxed cell volume (Equation (5)).

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