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ABSTRACT
Atomistic simulations are employed to investigate chemical short-range ordering in two body-centered cubic refractory multi-principal element alloys, HfMoNbTaTi and HfNbTaTiZr, and its influence on their ideal simple shear strengths. Both the alias and affine shear strengths are analyzed on the {110} and {112} planes in the two opposing ⟨111⟩ directions. In both quinary alloys, local ordering of NbNb, TaTa, HfNb, HfTa, and NbTa is preferred as the annealing temperature decreases from 900 to 300 K. The pair that achieves the highest degree of local ordering is TiTi in HfMoNbTaTi and HfTi in HfNbTaTiZr. Subject to the affine shear, these alloys yield by first phase transformation at the most likely pairs followed by deformation twinning at those sites.

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I. INTRODUCTION
Refractory multi-principal element alloys (RMPEAs) have been identified as promising candidate materials for aerospace propulsion systems, land-based gas turbines, nuclear reactors, heat exchanger tubing, and the chemical process industry. These materials consist of at least three metallic elements with equal- or near-equal molar ratio with most or all constituent elements being refractory metals. Two equal-molar quinary RMPEAs, HfMoNbTaTi and HfNbTaTiZr, possess outstandingly high room temperature (RT) strengths. Take the compressive yield strength as an example. It is 1369–1713 MPa for HfMoNbTaTi and 900–1073 MPa for HfNbTaTiZr. Unlike pure refractory metals, many RMPEAs can retain ultra-high strengths over a broad range of elevated temperatures. For example, the compressive yield strength of HfMoNbTaTi decreases from 1369 MPa to 699 MPa (i.e., −49%) when the temperature increases from RT to 1473 K. The percentage decrease is smaller than those in pure refractory metals. For example, in Nb and Ta, the ultimate tensile strengths at RT, 290 and 441 MPa, respectively, decrease to 65 and 106 MPa at 1473 K. The relative change is −78% in Nb and −76% in Ta.

The high temperature strengths of RMPEAs, e.g., 699 MPa for HfMoNbTaTi at 1473 K, are impressive, when compared to those of six currently used Ni-based superalloys, 115–185 MPa at the same temperature. The other alloy, HfNbTaTiZr, is one of the few RMPEAs that has sufficient RT tensile ductility, being 11%–25%. The ductility of its subsets is also high, e.g., HfNbTa (10%), HfNbTaTi (11%), Hf27.5Nb5Ta5Ti35Zr27.5 (23%), HfNbTiZr (14%–15%), HfTa0.5TiZr (27%), and NbTaTi (19%).

One characteristically intriguing feature of RMPEAs is their lack of chemical long-range ordering. In the meantime, many RMPEAs have been found to exhibit chemical short-range ordering (CSRO) that influences dislocation dynamics in these alloys. Using atomistic simulations in HfNbTaZr, the slip resistance of an edge dislocation was found to increase with CSRO. In another RMPEA, NbTiZr, greater CSRO led to slightly lower shear stress to move a screw dislocation. Atomistic simulations have been
used widely for strength studies in body-centered cubic (BCC) MPEAs but mostly for non-RMPEAs and with a few exceptions for RMPEAs, including MoTaWZr, to calculate their tensile and compressive strengths, and AlMoTaW and MoNbTaW to determine their compressive strengths.

In this article, using atomistic simulations, we investigate the effect of CSRO on the ideal shear strengths of HfMoNbTaZr and HfNbTaTiZr. We show that in five atomic pairs—NbNb, TaTa, TiTi, and ZrZr—and the cross interactions among these elements are based on the formulations by Johnson and Zhou. The resulting interatomic potentials built for the HfMoNbTaTi and HfNbTaTiZr RMPEAs are referred to hereinafter as the alloy potentials. Based on them, we construct two A-atom potentials, which provide mean-field representations of the RMPEAs, resulting in two artificial pure metals, denoted as HfMoNbTaTi4 and HfNbTaTiZr4, respectively. Except the HfNbTaTiZr alloy potential, all four potentials are newly developed here. They can be downloaded at https://github.com/shuozhixu/APLmater_2022.

To assess the accuracy of these potentials, we performed density functional theory (DFT) calculations for the lattice parameters (a0) and effective BCC elastic constants (C11, C12, C44) for the random structures of the two RMPEAs and compared these quantities with those from the alloy potentials. The atomistic and DFT calculations here are performed via Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) and Vienna Ab initio Simulation Package (VASP), respectively, following our previous work. We also compare the alloy potential-based results with available DFT or experimental data in the literature. In Table I, it is found that the alloy potentials generally well predict the structural parameters compared with the present and prior DFT results. In particular, our HfNbTaTiZr alloy potential, which yields C11 = 111.83 GPa, performs better than a modified EAM potential, which yields a much smaller C11 (69.09 GPa) than experimental (116 GPa) and DFT values (118.27–124.4 GPa).

### B. Ideal shear strength

Generally, the ideal shear strength is the minimum stress needed to plastically deform an infinite defect-free material and is an upper bound to the shear stress of the material. It is not related to the shear strength of a material that already contains defects. There are two types of ideal shear: the alias shear and the affine shear. The alias shear strength is related to the potential energy to displace two crystalline halves across a given slip plane. The affine shear strength allows the entire crystal to deform to accommodate the homogeneously applied shear. In each type, the applied shear can be either a pure shear or simple shear. These different types of shear calculations have been compared for pure face-centered cubic (FCC) metals and FCC MPEAs, revealing that (i) the simple shear strength is higher than the pure shear strength and (ii) the affine shear strength is higher than the alias one. The first statement was found to hold in pure BCC metals. However, the affine and alias shear strengths have not been compared in any pure BCC metals or RMPEAs. Here, we consider both alias and affine shear strengths in simple shear. Compared with the pure shear strength, the simple shear strength is more closely related to the slip resistance for a dislocation when the shear plane is selected as the glide plane. Between the two RMPEAs studied here, dislocations were experimentally investigated only in HfNbTaTiZr, suggesting that screw dislocations on [110] and [112] planes are prevalent. Our recent atomistic modeling work in six RMPEAs also showed that these two planes are operative during plastic deformation. Therefore, two shear planes, [110] and [112], are considered in this work.

### 1. Simulation cells for the RMPEAs

We first construct special quasi-random structures (SQSs) in which the five elements are randomly distributed using ATAT.
The crystallographic orientations are always (110), (112), and (111) along x, y, and z directions, respectively. Five different simulation cell sizes (A–E), summarized in Table II, are considered. For each RMPEA, there are two size A, two size B, and two size C cells, in which either \( L_x \) or \( L_y \) is the largest cell edge length. For the larger cells considered, size D and size E, there is only one size.

Two size C and one size D cells are employed to generate structures with CSRO. We first determine the chemical potential differences between Nb and the other five elements under the semi-grand-canonical (SGC) ensemble at 1500 K via the hybrid MD/MC technique using a small cubic cell containing 2000 atoms. The values obtained are summarized in Table S1 in the supplementary material. Next, based on the values of structural parameters of size D structures with CSRO, and so the equilibrium configurations with the equal-molar MPEAs. In a completely random structure, \( a_{ij} = 0 \) for all \( i \) pairs. A tendency for segregation or local ordering corresponds to a positive \( a_{ij} \) for pairs of the same species (i.e., \( i = j \)) or a negative \( a_{ij} \) for those of different species (i.e., \( i \neq j \)). In either case, a higher \( a_{ij} \) magnitude suggests a higher degree of CSRO.

In what follows, we use “number+K-MD/MC” to denote the structure obtained by hybrid MD/MC simulations at a specific annealing temperature. For example, “600KMDMC” represents the structure created by hybrid MD/MC simulations at 600 K. The values of structural parameters of size D structures with CSRO are provided in Table I. In general, the presence of CSRO influences \( c_{11}^{∥}, c_{12}^{∥}, \) and \( c_{44}^{∥} \) much more than it does \( a_{0} \).

### 2. Alias simple shear strength

The alias simple shear strength, \( T_{a,s} \), is the maximum stress for the sliding between two adjacent atomic planes along a certain direction. In BCC metals, \( T_{a} \) has been related to the generalized stacking fault energy (GSFE) curve \( \gamma_{gsf}^{α} \). All eight random structures and three structures with CSRO are used to calculate \( \gamma_{gsf}^{α} \). A 20 Å thick vacuum is added, along the \( x \) and \( y \) directions, respectively, to the (110) and (112) cells (Table I). Along all directions, periodic boundary conditions (PBCs) are applied. The top atomic planes are displaced by \( d \) with respect to the bottom ones along the \( z \) direction. Following each displacement, energy minimization is performed, in which the top two and bottom two atomic planes are fixed while the remaining ones are allowed to move along the \( x \) and \( y \) direction, respectively, in (110) and (112) cell. A GSFE curve is then obtained as a function of \( d \) from 0 to \( \sqrt{3}a_{0}/2 \). More details of the GSFE calculations in RMPEAs can be found in Refs. 36 and 41, which were focused on random solid solutions.

The procedure is repeated for several parallel planes with distinct atomic arrangements. We obtain 80 \( \gamma_{gsf}^{10} \) curves and 100 \( \gamma_{gsf}^{112} \) curves for each cell in each RMPEA. Each GSFE curve exhibits a single peak value, called the unstable SFE \( \gamma_{usf} \), i.e.,

\[
\gamma_{usf} = \max(\gamma_{gsf}(d)).
\]

In pure BCC metals, the (112) plane exhibits a geometric asymmetry in shear resistance in the twinning (soft) and anti-twinning (hard) (111) directions. In RMPEAs, the fluctuations in composition across the glide plane can induce a chemical asymmetry in the resistance to shear between positive and negative (111) directions, even for the (110) plane. Here, we use \( T_{d,s} \) to denote the soft sense and \( T_{d,h} \) the hard sense, as defined by

\[
T_{d,s} = \max \left| \frac{\partial \gamma_{gsf}(d)}{\partial d} \right|, \quad 0 \leq d < \sqrt{3}a_{0}/4,
\]

\[
T_{d,h} = \max \left| \frac{\partial \gamma_{gsf}(d)}{\partial d} \right|, \quad \sqrt{3}a_{0}/4 \leq d < \sqrt{3}a_{0}/2.
\]

### 3. Affine simple shear strength

To calculate the affine simple shear strength \( T_{a} \), four size D cells—one SQS and three structures with distinct CSRO—are adopted for each RMPEA. Size D, instead of size C, is chosen because it is sufficiently large to accommodate possible defect nucleation and

| Size | A | B | C | D | E |
|------|---|---|---|---|---|
| 110  | \( L_x \) | 270.56 | 272.03 | 271.56 | 135.77 | 271.52 |
|      | \( L_y \) | 8.1 | 24.33 | 32.44 | 137.84 | 275.66 |
|      | \( L_z \) | 2.89 | 20.07 | 31.54 | 137.61 | 272.29 |
|      | \( A_{xz} \) | 0.23 | 4.88 | 10.23 | 189.68 | 750.59 |

| 112  | \( L_x \) | 4.66 | 23.41 | 32.77 | 135.77 | 271.52 |
|      | \( L_y \) | 275.84 | 275.56 | 275.75 | 137.84 | 275.66 |
|      | \( L_z \) | 2.89 | 20.07 | 31.54 | 137.61 | 272.29 |
|      | \( A_{xz} \) | 0.13 | 4.7 | 10.34 | 186.83 | 739.32 |
FIG. 1. Atomistic structures of size C cells for two RMPEAs with or without CSRO. For each RMPEA, the top four snapshots are the projections of the structures onto the yz plane. Visualization is done in OVITO.

III. RESULTS AND DISCUSSION

A. Size effects in the alias shear strength

Calculating $\gamma_{ud}$ and $T_{ud}$ requires selecting a cross-sectional area $A$. Figure 2 shows the effect of $A$ on the average ($\bar{T}_{al}$) and standard deviation in $T_{al}$ ($S_{al}$) for two RMPEAs. For the broad range of sizes considered, $A$ is found to have a small effect on $\bar{T}_{al}$ and decreases linearly with increasing $A$. However, $S_{al}$, on the other hand, is affected by $A$ and increases with increasing $A$. These size effects are similar to those found in a study on the intrinsic SFE in FCC equal-molar FeNi binary and unequal-molar CrFeNi MPEA.

For reference, $T_{al}$ and $T_{ud}$ of five pure metals—two A-atom ones, HfMoNbTaTi, HfNbTaTiZr, and three BCC constituents, Mo, Nb, and Ta—are also calculated using similar procedures. Results of the last three metals are summarized in Table S2 in the supplementary material.
The size effect is also examined for the quinaries with CSRO by repeating the \( \gamma_{\text{usf}} \) and \( T_{\text{al}} \) calculations for structures of sizes C and D. Since the chemical ordering is short-range, the influence of changing CSRO is expected to diminish for the larger \( A \). We find that for the random and 900KMDMC cases, the values are the same between the two sizes. For 600KMDMC and 300KMDMC, the effects of CSRO are slightly subdued with the larger size D. Apart from this, CSRO does not change the fact that the quinaries have lower \( \bar{\gamma}_{\text{usf}} \) and \( \bar{T}_{\text{al}} \) values than HfNbTaTiZr, and that the standard deviation for size D is lower than that for size C. The last point is demonstrated in Fig. S4 in the supplementary material.

**B. CSRO**

The WC parameters for all possible pairs in both quinaries are provided in Tables S3 and S4 in the supplementary material. At the lowest annealing temperature of 300 K, results for HfNbTaTiZr show that NbNb, TaTa, HfNb, HfTa, NbTa, NbZr, TaZr, and TiZr pairs are likely, while in HfMoNbTaTi, the NbNb, TaTa, TiTi, HfMo, HfNb, HfTa, MoNb, MoTa, and NbTa pairs would tend to segregate. In general, the median of the absolute WC parameter values is higher for HfNbTaTiZr than for HfMoNbTaTi. In the 300KMDMC case, for instance, the median is 0.224 for HfMoNbTaTi compared to 0.242 for HfNbTaTiZr. Figure 3 shows the evolution of the five most significantly favored elemental pairs in the two RMPEAs, as the annealing temperature decreases. The most favored pair is TiTi and HfTi, respectively, in HfMoNbTaTi and HfNbTaTiZr.

Between the two RMPEAs, the CSRO in only HfNbTaTiZr has been previously investigated. Experiments have found segregation of the NbTa pair between 773 and 1073 K\(^9,13,73–76\) and the HfTa pair between 873 and 1073 K.\(^77\) At a high temperature of 2773 K, \textit{ab initio} MD simulations found that CSRO is absent.\(^78\) Based on a modified EAM potential,\(^34\) Huang \textit{et al.}\(^79\) showed that four unlike atomic pairs tend to segregate at 800 K: HfTi, HfZr,
the annealing temperature decreases from 600 to 300 K, it is not consistent for the two shear planes. For example, when

In HfMoNbTaTi, the influence of CSRO is more noticeable, yet increases in the hard sense, while decreasing in the soft sense.

The only two discrepancies between the present work and first principles calculations pertain to ZrZr and HfZrTa. These are likely owing to the difference in the interatomic potential or the cell size used.

C. CSRO effects on shear strength

Figure 4 presents both $\tilde{T}_{\text{af}}$ and $T_{\text{af}}$ of two RMPEAs with CSRO attained at three different annealing temperatures. The evolution of the strengths in the hard and soft senses is tracked individually. We include for reference the strengths of the A-atom versions of these RMPEAs, which are found to provide a good estimate of $T_{\text{af}}$, but not $T_{\text{di}}$, with respect to the random alloy.

We first discuss the alias shear strength. $T_{\text{di}}$ values for HfMoNbTaTi are higher than those for HfNbTaTiZr, a reflection of the fact that Mo is stronger than Zr. For both quinaries, in the case of A-atom pure metal and random alloy, which have no CSRO, $T_{\text{di}}$ on the (112) plane is higher than that on the (110) one. In HfNbTaTiZr, with an increasing CSRO, $T_{\text{di}}$ only slightly increases in the hard sense, while decreasing in the soft sense. In HfMoNbTaTi, the influence of CSRO is more noticeable, yet it is not consistent for the two shear planes. For example, when the annealing temperature decreases from 600 to 300 K, $T_{\text{di}}$ on the [110] plane decreases, while that on the [112] plane increases. The anisotropy in CSRO effects, exhibited for different senses or planes, is intriguing. It may be a result of the anisotropic clustering/segregation during the annealing. For both quinaries, increasing the CSRO levels tends to increase the asymmetry between the hard and soft senses. Overall, the CSRO effects on $T_{\text{di}}$ are relatively weak. On the other hand, prior atomic simulations showed that $T_{\text{af}}$ is positively correlated with the local slip resistance in pure refractory metals and RMPEAs. These suggest that the CSRO effects on slip resistance are weak in RMPEAs, consistent with prior atomic studies.

Next, we discuss the affine shear strength. $T_{\text{af}}$ values for the A-atom pure metals and RMPEAs exhibit the expected anisotropy with the [112] strength in the hard sense being greater than the [110] strength and both greater than the [112] strength in the soft sense. Moreover, compared with $T_{\text{di}}$, $T_{\text{af}}$ is less sensitive to the bulk composition. However, both quinaries display similar trends in $T_{\text{af}}$ with increasing CSRO level. For example, when the annealing temperature decreases from 900 to 300 K, $T_{\text{af}}$ increases in both RMPEAs.

The mechanism of affine shear deformation is not concentrated to a single plane in the crystal and in fact could be unrelated to dislocation motion. Thus, its deformation mechanisms are completely different from that presumed by alias shear. For example, subject to the affine simple shear, both Mo and Nb yield via the homogeneous nucleation of twins, as shown in Fig. 5(a). The same yielding mechanism was reported in tensile loading of a Mo single crystal using the same interatomic potential employed here. In Ta, as well as the two A-atom materials, yield occurs first by a BCC-to-FCC phase transformation (PT) followed by homogeneous nucleation of twins, as shown in Fig. 5(b). A similar BCC-to-FCC PT was reported in shearing of Fe using atomistic simulations. Both RMPEAs, with or without CSRO, yield first by a BCC-to-FCC PT in local regions followed by twinning in those same regions. In HfMoNbTaTi, Ti atoms tend to form clusters with homogeneous nucleation of twins, as shown in Fig. 5(c). Likewise, in HfNbTaTiZr, the HfTi pair tends to segregate and initial local PT occurs in these HfTi-rich regions. Between the two RMPEAs, deformation twinning was experimentally observed in HfNbTaTiZr, but not yet in the other alloy.

CSRO effects on deformation of RMPEAs have been studied previously only for polycrystals using experiments (exp) or MD simulations, where CSRO was found to increase the tensile strength in HfNbTaTiZr (exp) and MoNbTaW (MD) as well as hardness and compressive strength in HfNbTaZr (exp). Although shear deformation was not explicitly studied, results from uniaxial deformation indicate that CSRO likely increases $T_{\text{af}}$. Recent atomistic simulations in FCC CoCrNi MPEA have found that CSRO promotes the

![Figure 4](https://example.com/figure4.png)

**FIG. 4.** (a) Alias simple shear strength and (b) affine simple shear strength, in structures of size D in two RMPEAs with or without CSRO. “h” and “s” denote hard and soft senses, respectively.
FCC-to-BCC PT, which suggests that it may decrease $T_{af}$. CSRO was also shown to increase $\gamma_{usf}$ in two BCC RMPEAs, MoNbTi and TaNbTi, suggesting that it might promote $T_{af}$. Here, our simulations show that higher levels of CSRO have different effects on $T_{af}$ and $T_{al}$ in RMPEAs. For both strengths, the CSRO effects are not influenced by either the cross-sectional area or temperature, a conclusion that can be reached if one compared Fig. 4 with Fig. S5 in the supplementary material.

Finally, for the same sense on the same plane in the same RMPEA, $T_{al}$ is plotted with respect to $T_{af}$ in Fig. S6 in the supplementary material. It is shown that the two strengths are loosely correlated, with higher $T_{al}$ corresponding to higher $T_{af}$ and vice versa. The weak relationship may be expected since the mechanisms accommodating deformation in each type are different, in either pure metals or RMPEAs.

IV. CONCLUSIONS

In this article, we conduct atomistic simulations to calculate the alias ($T_{al}$) and affine ($T_{af}$) ideal simple shear strengths in two quinary RMPEAs, HfMoNbTaTi and HfNbTaTiZr, with or without CSRO. The strengths in two opposing (111) directions on both [110] and [112] planes are calculated. For reference, the same strengths of the constituent elements Mo, Nb, and Ta, as well as hypothetical $A$-atom homogeneous versions of HfMoNbTaTi and HfNbTaTiZr, are also calculated. The main findings are summarized as follows:

1. The interatomic potentials for both RMPEAs are validated by comparing the corresponding lattice parameters and elastic constants against those from DFT and experimental data.
2. The size of the cross-sectional area $A$ does not affect the average $T_{al}$ much. However, a smaller $A$ increases the standard deviation in $T_{al}$.
3. The two RMPEAs possess much lower $T_{al}$ and $T_{af}$ than the constituent BCC metals: Mo, Nb, and Ta.
4. In both RMPEAs, five atomic pairs, NbNb, TaTa, HfNb, HfTa, and NbTa, tend to segregate. The degree of CSRO increases with decreasing annealing temperature. The most likely pairing is TiTi in HfMoNbTaTi and HfTi in HfNbTaTiZr.
5. Subject to affine simple shear deformation, the two RMPEAs yield by two steps: first a BCC-to-FCC PT followed by twinning. In HfMoNbTaTi, the PT preferentially occurs at the boundaries of Ti clusters, whereas in HfNbTaTiZr the PT tends to initiate in the HfTi-rich regions.

SUPPLEMENTARY MATERIAL

See the supplementary material for information as referred to in the main text.
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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Shuozi Xu: Conceptualization (equal); Data curation (lead); Formal analysis (lead); Investigation (lead); Methodology (lead); Visualization (lead); Writing – original draft (lead); Writing – review & editing (equal). Wu-Rong Jian: Methodology (supporting); Resources (supporting); Validation (lead); Writing – review & editing (supporting). Irene J. Beyerlein: Conceptualization (equal); Funding acquisition (lead); Supervision (lead); Writing – review & editing (equal).

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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