A ductility-strength metric for chemically complex alloys

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Abstract

Local lattice distortions (LLD) – relative to average (x-ray) lattice positions – are expected in multi-principal element alloys (MPEAs) due to the varying complex chemical environments. We suggest a dimensionless metric to characterize ductility in MPEAs using LLD. With its innate quantum-mechanical origins, ductility is clearly affected by LLD arising from increased atomic charge transfer due to electronegativity differences in each local environment (often designated by valence electron count (VEC)). To test this metric, we chose body-centered cubic (bcc) refractory alloys that exhibit a range of ductility-brittleness. The metric was established by combining the weighted-average VEC (ΔwVEC) and intrinsic parameters (Δu, √[Δu]²) related to distortion from the average lattice. The electronic-structure results were calculated using density-functional theory (DFT) methods. The quantitative rank ordering of ductile-to-brittle MPEAs shows good agreement with recent mean-field estimates and experiments. Our results permit a quick ductility assessment to guide the design of more ductile high-temperature MPEAs, and potentially accelerated further if combined with machine-learning.

Keywords: MPEAs, DFT, Ductility, Strength, Lattice distortion, Electronic structure

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Introduction

Since the concept of multi-principal element alloys (MPEAs) was proposed [1,2], numerous systems have been developed to enhance high-temperature phase stability that expands the design prospects for new alloys [3-22]. Refractory MPEAs (R-MPEAs) are a relatively new class of single-phase materials based on body-centered cubic (bcc) refractory elements often mixed with low-density bcc metals [23,24]. These alloys have received more attention compared to other group of metallic alloys due to their attractive properties, such as weak temperature dependence of yield strength, which is about 400 MPa near 1600°C [25,26]. These MPEAs, in general, have low ductility even in compression, which is intrinsic to bcc metals, so such behavior goes beyond MPEAs [27,28]. Moreover, no correlation has been found between ductility and strength. To emphasize this, yield stress is higher in refractory MoWNbTa (1 GPa), MoNbTaTi (1.2 GPa), NbTaTiW (1.8 GPa), and MoWNbTaV (1.25 GPa) but ductility remains very low in all cases [29,30]. This suggests that R-MPEAs are quite brittle with relatively sharp brittle-to-ductile transition with increasing temperatures.

Lilensten et al. [31] and Huang et al. [32] proposed the idea of metastability-engineering to improve the ductility in bcc-refractory MPEAs. This idea was utilized for steels [33,34] and for Ti-based bcc [35,36] and fcc [37] MPEAs to enhance uniform tensile ductility [38]. In MPEAs, solid-solution strengthening affected by local lattice distortions (LLD) has been invoked to rationalize the high strength, where mismatch in atomic sizes and elastic moduli are expected to retard dislocation motion – a standard mechanism [39-43]. There have been a number of theoretical studies to provide some understanding of yield stress, e.g., [44,45]. However, the literature related to theoretical/numerical approaches to characterize ductility in MPEAs remain sparse [30,46]. This gap in the literature to understand the quantum origin of key mechanical properties such as ductility needs to be addressed in order to aid the design of new alloys with superior properties. As such, it is timely to explore new lines of study.

Here, we hypothesize that the ductility in bcc MPEAs has a quantum origin controlled by intrinsic features, such as chemical disorder and parameters controlling lattice distortions. The transition from high-to-low ductility (or vis-à-versa) is expected to have strong connection to these nanoscale manipulations. As such, we propose a dimensionless metric for bcc random alloys to characterize ductility via quantities derived from atomic displacements \( \Delta u, \sqrt{\langle \Delta u \rangle ^2} \) relative to equilibrium atomic positions, obtained by minimizing the Hellmann-Feynman forces using density-functional theory (DFT) calculations within a Super-Cell Random APproximates (SCRAPs) that mimic appropriate configurations for random alloys. A SCRAP is constructed as an optimal supercell of fixed size (number of sites) with physically most relevant atomic short-range order (here we focus on homogeneous random alloys, where pair correlations are optimized to zero to the third-neighbor shell around every site). From each relaxed supercell, we extract displacements and derived quantities to construct a dimensionless ‘LLD’ metric to successfully characterize
ductility in bcc refractory MPEAs, as supported by experimental validation. This work offers a pathway to develop novel R-MPEAs with improved strength-ductility – critical for high-temperatures applications.

**Methodology**

The total-energy calculations were performed using the DFT-based Vienna *ab initio* simulation package (VASP) [47] using projector-augmented waves (PAW) method [48,49]. The Perdew-Burke Ernzerhof (PBE) [50] DFT exchange-correlation functional is used for non-spin-polarized generalized gradient approximation (GGA). The kinetic energy cutoff of 500 eV is employed for the plane-wave basis. The Monkhorst-Pack scheme for Brillouin zone integration was carried out using $5 \times 5 \times 5$ k-points [51] meshes. The convergence threshold for energy is $10^{-5}$ eV, while the symmetry-unrestricted optimization for the geometry is performed by employing a conjugate-gradient scheme until the residual force on each atom is less than 0.01 eV/Å. A Super-Cell Random Approximates (SCRAPs) supercell of a 60-atom ($5 \times 3 \times 2$) and 90-atom ($5 \times 3 \times 3$) were used to mimic the homogeneously random MPEAs, as generated using a Hybrid Cuckoo Search optimization method [52]. The in-depth understanding of the local lattice-distortion and its correlation with ductility and yield-strength gained through this investigation is expected to provide an advance for the design of R-MPEAs for high-temperature applications.

**Ductility Metric**

Improving ductility of R-MPEAs has been an impediment for useful application. To address this challenge, we propose a dimensionless metric that uses scalar/vector atomic displacements extracted from a fully relaxed random supercells using first principles DFT methods. These parameters are a building block for our surrogate model created from positional imbalance around ideal-site symmetries. The *subset of local structural parameters* (i.e., an average LLD ($\Delta u$) and vector ($L_{2,1}$) norm of atomic displacements $\sqrt{\langle \Delta u(x,y,z)^2 \rangle}$ from all atoms in supercell) derives from assuming that increased charge sharing, and lattice relaxation increases bond strength and, thereby, the mechanical properties of MPEAs.

The new metric “LLD” is dimensionless and defined as the ratio of average local lattice displacement ($\Delta u$) and square root of vector sum of lattice displacements $\sqrt{\Delta u(x,y,z)^2}$ for each relaxed MPEA supercell. The metric ‘LLD’ for MPEAs is defined as follows:

$$LLD = \frac{\Delta u \Delta W_{VEC}}{\sqrt{\langle \Delta u (x,y,z)^2 \rangle}},$$  

where

$$\begin{cases} 
\text{LLD} \leq 0.3 \; \text{(ductile)} \\
\text{LLD} > 0.3 \; \text{(brittle)} 
\end{cases}$$

and $\Delta W_{VEC} = \text{VEC}_{\text{MPEA}} - [\text{VEC}_{\text{max}} - \text{VEC}_{\text{min}}]$ is the weighted VEC, i.e., the difference between VEC of MPEA with respect to max-bcc VEC$_{\text{max}}$ and min-bcc VEC$_{\text{min}}$ values. The weighted average of VEC
difference of MPEAs in Eq. (1) was defined to remove the superficial dominance of . The $\Delta u (x, y, z)$ is distance between displaced atoms from high-symmetry points between relaxed and ideal atomic positions in the supercell due to local lattice mismatch, and $\sqrt{[\Delta u(x,y,z)]^2}$ is a mean-value derived from vector displacements of all atoms in the relaxed supercell.

**Results and discussion**

To test the metric, we studied bcc-refractory (ternary, quaternary, quinary) MPEAs, such as Senkov alloys [6], and compared with recent work of Curtin, et al. [38]. We generated a large enough supercell for each case, where the volume (lattice constant) and atomic (co-coordinates) positions were fully optimized. In particular, we used 60-atom (5x3x2 bcc cubes) SCRAP for ternary/quaternary and 90-atom (5x3x2 bcc cubes) SCRAPs for quinary systems. We plot the “LLD” metric with respect to average atomic displacement (Fig. 1a), and $\Delta VEC$ (Fig. 1b) of MPEAs. While LLD is by definition linear in $\Delta u$, it is renormalized by $\Delta VEC/\sqrt{[\Delta u(x,y,z)]^2}$. In Fig. 1a, we find a linear correlation between $\Delta u$ and LLD, with clear separation at 0.30 (LLD along y-axis) between experimentally known ductile and brittle behavior, as tabulated in Table 1. A clear range in VEC ($\Delta VEC=3$), $\Delta u$ (0.05 Å), and LLD (0.3) was seen in Fig. 1a,b, although not as evident for static displacement, $\Delta u=0.05$ Å. This suggests that rather than severe lattice distortion, the generalized dimensionless LLD metric including the effect of electron counts is more physical in characterizing ductility of MPEAs, which is caused by charge-transfer effect on mean-value of vector displacements.

The higher $\Delta u$ in Fig. 1a shows an inverse correlation with ductility. In literature, LLD is connected to strength of alloys, but this does not guarantee ductility, especially, bcc refractory MPEAs that are known to be mostly brittle. Moreover, larger LLD in distorted refractory lattices is expected to induce large local elastic-stress fields. The interaction of mobile dislocations with the local stress fields may hinder dislocation glide during deformation, which accounts for the large dislocation density during plastic deformation [53,54]. Recently, Lee et al. [54] highlighted this by comparing change in dislocations density near the $\{110\}$- and $\{200\}$-oriented planes in as-cast versus homogenized MPEAs. Thus, when characterizing strength, we need to look at a reasonable trade-off between ductility and strength during the design of alloys using expensive computational schemes. However, our predicted ductility from the LLD metric shows extremely good agreement when compared with other theory and experiments [55] for known bcc MPEAs, see Table 1.
Figure 1. Dimensionless LLD metric (Eq. 1) versus (a) the magnitude of the vector atomic displacement from average lattice $|\Delta u(x, y, z)|$, and (b) the difference of VEC, where colored regions represent ductile (green) and brittle (red). The metric rank orders the ductility of bcc MPEAs (Eq. 2). The ductile-brittle behavior of 15 CALPHAD+ML selected MPEAs was assessed, and shown by red-squares (7), blue-diamonds (3), and cyan-triangles (5), where three symbols/color represent quinary Mo-Nb-Ti-V-W (7) and septenary Mo-Nb-V-Cr-Ta-W-Al (10) MPEAs.

The use of lattice-distortion parameters in determining the local atomic displacement for MPEAs are somewhat ambiguous. This possibly has to do with the definition of ‘local’ in relaxed atomic supercells, and its correlation with charge (calculated from DFT) or electronic configuration (valence electron count) with atomic sizes. However, we found a clear correlation between static displacement and effective electronic charges with LLD metric, see Fig. 1a. What is the origin of increasing displacement in MPEAs (e.g., charge, atomic size or both)? We found that the high LLD are induced mainly by atomic-size mismatch in MPEAs, which will reduce the deformability of alloy by hindering slip plane easy glide [54]. Figure 1a shows that LLD metric [Eq. 1 & 2] gives a reliable prediction of ductility (deformability).

The VEC has been connected to deformability of alloy, where lower VEC (<4.5) is expected to improve the ductility. We plot $\Delta$VEC vs LLD metric in Fig. 1b and found that the displacements in bcc MPEAs has more to do with atomic sizes than the charge or electron configuration of constituent elements. With each MPEA marked in Fig. 1b, the displacement or LLD metric increases with alloys having increasing at.% of elements with increasing VEC, such as Cr, Mo, or W. Along with a clear demarcation in LLD (=0.30), we also found a clear value in $\Delta$VEC that separates ductile behavior of MPEAs ($\Delta$VEC < 3.0) from brittleness ($\Delta$VEC > 3.0). We also found that ductile MPEAs fall in the area shaded in green, where Al/Ti/Zr are revealed as the main elements to drive bcc ductility. Our predictions match well with earlier reports that lower VEC improves the ductility [56,57].
Table 1. The proposed dimensionless distortion metric, LLD (Eq. 1) to characterize ductility in bcc refractories. LLD predictions from DFT are in good agreement with mean-field theory (MFT) [44] and experiments [6,49,58-63].

| MPEAs               | $\Delta u$   | $\sqrt{\Delta u^2}$ | $\Delta w_{VEC}$ | LLD | Curtin [MFT] | this work [DFT] |
|---------------------|--------------|----------------------|------------------|-----|---------------|-----------------|
| NbTiZr              | 0.0121       | 0.3505               | 2.33             | 0.081 | 1             | 3               |
| AlNbTaTi            | 0.0252       | 0.3873               | 2.25             | 0.146 | 2             | 7               |
| Nb$_{6.8}$Mo$_{1.4}$Ti$_{1.8}$ | 0.0116   | 0.5065               | 2.94             | 0.067 | 3             | 1               |
| Nb$_{7.0}$Mo$_{1.2}$Ti$_{1.8}$ | 0.0116 | 0.5065               | 2.96             | 0.068 | 4             | 2               |
| NbTaTi              | 0.0330       | 0.5549               | 2.67             | 0.159 | 5             | 5               |
| NbTaTiV             | 0.0319       | 0.6174               | 2.75             | 0.142 | 6             | 4               |
| MoNbTiV             | 0.0320       | 0.4833               | 3.00             | 0.199 | 7             | 8               |
| MoNbTaTi            | 0.0619       | 0.6446               | 3.00             | 0.288 | 8             | 10              |
| MoNbTaV             | 0.0484       | 0.7039               | 3.00             | 0.206 | 9             | 9               |
| NbTaTiW             | 0.0348       | 0.5866               | 3.00             | 0.178 | 10            | 6               |
| CrMoTaTi            | 0.1400       | 0.9394               | 3.25             | 0.484 | 11            | 14              |
| CrMoNbTi            | 0.1187       | 0.8657               | 3.25             | 0.446 | 12            | 13              |
| CrMoNbV             | 0.0739       | 0.6663               | 3.25             | 0.388 | 13            | 11              |
| MoNbTaWV            | 0.0591       | 0.5273               | 3.45             | 0.381 | 14            | 12              |
| MoNbTaW             | 0.1537       | 0.9500               | 3.54             | 0.566 | 15            | 15              |

Our LLD metric predictions are good agreement with recent work of Curtin et al. [44], where MoNbTaW (#14) and MoNbTaWV (#15) were predicted to be brittle with less than 3% ductility at RT under compression, while NbTiZr (#1) was predicted to be ductile. These predictions are good agreement with existing experiments that show ductility for NbTaZr [59] and brittleness for MoNbTaW and MoNbTaWV [6]. Furthermore, the LLD metric was used to assess the ductility/brittleness of 7 new quinary Ti-V-Nb-Mo-W MPEAs (Nb-rich, i.e., Nb >60 at.%), shown in Fig. 1 by red circles. Six MPEAs satisfy the LLD metric constraint out of seven, i.e., LLD $<0.3$ in Eq. 2, but only two of them (Mo$_{1.8}$Nb$_{0.4}$V$_{2.5}$W$_{1.5}$ and Mo$_{0.1}$Nb$_{6.4}$Ti$_{1.5}$V$_{27.4}$W$_{1.6}$) satisfy critical LLD and DVEC limit for a MPEA to be ductile.

In Figure 1a,b, we plot LLD metric calculated for 15 predicted MPEAs belong to Mo-W-Ti-V-W (7), Mo-Nb-Ta-V-W (3), and Cr-Mo-Nb-V-W (5) family, which are filtered from high-throughput CALPHAD and machine-learning models that satisfy high-temperature strength criteria (>300 MPa and 1300°C). Our analysis shows that 4 out of 15 MPEAs satisfy all ductility criteria, i.e., LLD $<0.3$, $2<\Delta VEC<3$, and $\Delta u<0.1$, and 6 of them satisfy LLD and $\Delta u$ criteria but fall above $\Delta VEC$ range. In contrast, the remaining 5 MPEAs were found to be brittle, i.e., they do not satisfy any of the criteria set for ductility.

The strength and ductility tradeoff in materials can be obtained after thermal treatment and/or thermo-mechanical processing by controlling the microstructure to remove defects. To understand this tradeoff using LLD metric, we plot in Fig. 2 the LLD and average atomic size for MPEAs in Table 1 with respect to experimental yield strength (YS) [64]. The trend between LLD and YS in Fig. 2a shows an
increase in strength with LLD up to 0.3 which then decreases with increase in LLD. This suggests that maximizing lattice distortion is not always a reason for increased strength, i.e., there is an optimal LLD range for tuning strength and ductility tradeoff in MPEAs. In Fig. 2b, the plot of YS as a function of atomic size shows a linear correlation, such that atomic size increases the strength in bcc MPEAs from associated larger lattice distortions, which also suggests that the increment of YS can be predicted.

**Figure 2.** Measured yield strength (GPa) for bcc MPEAs vs. LLD (a), and atomic size (b). Higher ductility in Fig. 1 connects with lower strength, shaded area in (a). MPEA strength decreases with increasing average atomic size (b).

**Lattice distortions**

Hu, et al. [65] has shown that elemental radii do not accurately characterize the lattice distortion from a change in local environment, as distortions (and related properties) are strongly dependent on local chemical environment in MPEAs [52,66]. Moreover, the electronegativity difference of elements was found to correlate well with the mechanical properties [67], rather than Hume-Rothery size effect [68] and data-driven approaches [69]. To understand the effect of chemical complexity (alloying and environments) on local lattice distortion, we compare in Fig. 3 for three fully-relaxed quaternaries AlNbTaTi, VNbTaTi, and CrMoNbTi the relaxed SCRAP structures (Fig. 3a,d,g), local atomic displacement ($\Delta u$) along (x,y,z) in Fig. 3b,e,h, and the change in local atomic charges from varying neighbor environments (Fig. 3d,f,i).

**Figure 3b,e,h** illustrates the likelihood of an atomic site to be displaced (compressed or elongated) based on alloying species, their electronegativities, and atomic-sizes in AlNbTaTi, NbTaTiV, and CrMoNbTi MPEAs. The bond-length analysis of Nb and Ti (see Fig. A1) that are common in all three MPEAs analyzed in Fig. 3 found strong elongation in Nb-X bond-length when found in an environment of
Al and Nb in particular, while Nb-X bonds show compression or no change in CrNbTaTi compared to unrelaxed structures. Similarly, Ti-X bond lengths show weak elongation in NbTaTiAl and NbTaTiV, while Ti-X shows weak compression or no change in CrNbTaTi. This Nb-X and Ti-X elongation and compression of bond-lengths are also reflected in volume change in three MPEAs, where $V_{AlNbTaTi} (17.3 \text{ Å}^3$/atom$) > V_{NbTaTiV} (16.6 \text{ Å}^3$/atom$) > V_{CrNoNbTi} (15.4 \text{ Å}^3$/atom$)$. To be more specific, the homoatomic pairs, i.e., Nb-Nb and Ta-Ta, are atoms with large radii, thus, these are mostly compressed, while the homoatomic pairs of Ti-Ti and V-V are the smaller size atoms with significant elongation in MPEAs. The idea of bond elongation or compression based on alloying elements and their intrinsic characteristic is reflected through absolute lattice displacement in Fig. 3b,e,h. The change in average bond lengths is also related to enhanced charge-transfer due to varying chemical interactions of the principal elements in MPEAs.

The order of elemental electronegativities ($\chi$) on the Allen scale for solids is Nb (1.17), Ta (1.30), Cr (1.33), Mo (1.38), Ti (1.40), Al (1.52), and V (1.62). So, for NbTaTiAl $\chi_{Nb} < \chi_{Ta} < \chi_{Ti} < \chi_{Al}$, NbTaTiV $\chi_{Nb} < \chi_{Ta} < \chi_{Ti} < \chi_{V}$, and CrMoNbTi ($\chi_{Nb} < \chi_{Cr} < \chi_{Mo} < \chi_{Ti}$). Clearly, CrMoNbTi has the most elements with lower affinities for pulling charge from their neighbors, i.e., least distortion expected due to charge transfer, as is reflected in Fig. 3c,f,i. Moreover, charge analysis in Fig. 3c,f,i indicates both $\chi$ and $\Delta u$ due to atomic-size are strongly correlated with charge-transfer ability of alloying elements, which is quantified in our LLD metric that combines distortion parameters ($\Delta u$ and $\sqrt{\Delta u^2}$) with change in VEC in electronically distinct MPEAs.
Figure 3. The plot of relaxed SCRAPs, local lattice displacement, and effective charge transfer activity in (a-c) AlNbTaTi (high ductility), (d-f) NbTaTiV (low ductility), and (g-i) CrMoNbTi (no ductility).

Charge density analysis: The relationship between ductility and strength can further be understood from the charge density difference ($\Delta \rho$) between two MPEAs that reveals the nature of bonding and charge transfer. Thus, for three MPEAs, we analyzed the $\Delta \rho$ of three MPEAs that show high-ductility (AlNbTaTi), low-ductility (NbTaTiV), and no-ductility/brittle (CrMoNbTi), see Fig. 1 and Table 1. The $\Delta \rho_{CrMoNbTi-AlNbTaTi}$ in Fig. 4a shows increased charge transfer near Al in AlNbTaTi, while Cr-based CrMoNbTi shows almost no charge activity at/near Cr. The increased charge near/at Al can be attributed to large Al electronegativity ($\chi = 1.52$) compared to Nb- or Cr-based MPEAs. Also, increased charged activity or metallic interaction introduced by Al arises from delocalized 3s-3p electrons, while the increased charge activity at/near Ta ($4d^35s^2$) is due to larger atomic size. This suggests multiple mechanisms that are responsible for improved ductility in MPEAs. On the other hand, the effective charge transfer between brittle (CrMoNbTi) and weakly ductile (NbTaTiV) MPEAs in Fig. 4b shows improved charge activity, as shown by $\Delta \rho_{CrMoNbTi-NbTaTiV}$. Similar, the $\rho_NbTaTiV-AlNbTaTi$ in Fig. 4c shows much larger charge transfer activity, which further supports the increased lattice distortion for AlNbTaTi and NbTaTiV MPEAs, as shown in Fig. 3a-c and Fig. 3d-f. While CrMoNbTi in Fig. 3g-i shows very weak or no charge transfer, as is visible through local lattice distortion, mainly expected to originate from atomic-size effect.

For a 2D cross-section, we plot charge density for AlNbTaTi, NbTaTiV, and CrMoNbTi MPEAs (see Fig. A2), which shows reduced charge-transfer activity with increasing LLD metric that further establishes that charge-transfer is not necessarily responsible for the solid-solution strengthening.

Figure 4. Charge density difference (a) $\Delta \rho$ [CrMoNbTi – AlNbTaTi], (b) $\Delta \rho$ [CrMoNbTi – NbTaTiV], and (c) $\Delta \rho$ [NbTaTiV – AlNbTaTi] to emphasize a change in charge distribution (for an iso-surface value of 0.012 e/Å$^3$). Iso-
surfaces are positive (yellow) and negative (blue) charges. (d-f) Bond-length distribution about each element in fully relaxed 72-atom SCRAP (A [0-17]; B [18-35]; C [36-53]; D [54-71]) of MPEAs.

In Fig. 4d-f, we plot the average bond-length distribution (see also Fig. A3) around each species in high-ductility (AlNbTaTi), low-ductility (NbTaTiV), and brittle (CrMoNbTi) MPEAs. It shows that the nearest-neighbor interatomic distance of all pairs extends over a wide range in CrMoNbTi (Fig. 4f) compared to AlNbTaTi (Fig. 4d) and NbTaTiV (Fig. 4e), where Nb (36-53) and Ti (54-71) atoms show profound deviation from ideal sites, for increased (severe) lattice distortions. The large distribution of bond-length and DFT lattice distortion was found for CrMoNbTi, and the alloy was predicted to be the least ductile in our LLD metric, in agreement with experiments [30].

**Conclusion**

The peculiar characteristics of MPEAs has produced several design strategies to achieve strength-ductility synergy [55, 70-74], permitting MPEAs to be used in advanced structural applications requiring high strength and high ductility. The characterization of alloys purely on the basis of lattice distortion may give an idea about higher strength but not ductility. Importantly, alloys with little ductility are not useful for technological applications, therefore, we need to look for a strength-ductility trade-off. The proposed LLD metric (Eq. 1) and limits (Eq. 2) plotted for bcc MPEAs in Fig.1 (and list in Table 1) shows that higher lattice distortion leads to poor ductility. As is well-known, bcc refractory MPEAs have higher strength and generally poor ductility. Here, our analysis provides useful guidelines that we should aim to optimize LLD metric and strength to achieve a sweet spot for strength and ductility. As we have shown, ductility in MPEAs is strongly correlated to local charge-transfer activity and lattice distortion, which can be tuned by chemical alloying. The charge-transfer activity and lattice distortion for MPEAs were quantitatively determined from first-principles DFT calculations. Our results provide a more fundamental understanding of local lattice distortion and charge-transfer effects on ductility of bcc MPEAs.

In conventional alloys with a regular lattice, dislocation movements need to overcome the Peierls friction or the lattice stress through a kink-pair mechanism [75]. However, increased lattice distortion and the resultant residual stress field in MPEAs may enable significant strengthening, [76,77] improving the yield-strength in MPEAs. To the contrary, our study suggests that increased lattice distortion is not necessarily good for ductility. The good combination of strength and ductility derives from increased lattice friction yielding mechanical features beyond those reported before for bcc alloys. The proposed metric was successful in rationalizing the ductility across a range of ternary, quaternary, and quinary MPEAs. The metric driven analysis is validated from existing experiments on refractory alloys permitting improved strength-ductility design trade-offs critical for high-temperatures applications. Finally, our study also provides physical insights into which principal elements are responsible for enhanced ductility, which can contribute to accelerating the development of high-ductility materials [78].
**Acknowledgements:** Authors acknowledge the U.S. Department of Energy (DOE) ARPA-E ULTIMATE Program through Project DE-AR0001427. RA also acknowledges NSF through Grant No. 2119103. The method (SCRAPs) development at Ames Laboratory was supported by the U.S. Department of Energy (DOE) Office of Science, Basic Energy Sciences, Materials Science & Engineering Division. Research was performed at Iowa State University and Ames Laboratory, which is operated by ISU for the U.S. DOE under contract DE-AC02-07CH11358. High-throughput DFT calculations were carried out in part at the Texas A&M High-Performance Research Computing (HPRC) Facility.

**Author Contributions:**
P.S. – Conceptualization, Method development, Data curation, Formal Analysis, Writing - original draft, Writing-review and editing. R.A.– Formal analysis, Writing-review and editing. D.D.J.– Formal analysis, Writing-review and editing.

**Appendix:**

![Graph](image)

**Figure A1.** (a) Nb-Nb, and (b) Ti-Ti bond-length compression and elongation in (a) AlNbTaTi, (b) NbTaTiV, and (c) CrMoNbTi due to change in chemical environment in MPEAs.
Figure A2. The charge density plot for (a) AlNbTaTi, (b) NbTaTiV, and (c) CrMoNbTi MPEAs ranked as ductile, weakly ductile, and brittle based on dimensionless LLD metric (see Table 1).

In Fig. A3, we also show the bond-length distribution of selected MPEAs, where AlNbTaTi with higher ductility shows smooth (Gaussian) bond-distribution compared to skewed (bimodal) distribution in medium and low ductility MPEAs (here NbTaTiV and CrMoNbTi).

Figure A3. The distribution of atomic bond-lengths, and (b) the minimum distance between the atomic surface from the maximum cut-off radius for the core region versus local atomic volume.

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