A Strategic Design Route to Find a Depleted Uranium High-Entropy Alloy with Great Strength

Weiran Zhang 1,2,†, Yasong Li 2,†, Peter K. Liaw 3,4 and Yong Zhang 2,4,5,*

1 Xi’an Rare Metal Materials Institute Co. Ltd., Xi’an 710016, China; zhangweiranruth@163.com
2 Beijing Advanced Innovation Center of Materials Genome Engineering, State Key Laboratory for Advanced Metals and Materials, University of Science and Technology Beijing, Beijing 100083, China; songli19@sina.com
3 Department of Materials Science and Engineering, The University of Tennessee, Knoxville, TN 37996, USA; pliaw@utk.edu
4 Qinghai Provincial Key Laboratory of New Light Alloys, Qinghai Provincial Engineering Research Center of High Performance Light Metal Alloys and Forming, Qinghai University, Xining 810016, China
5 Shunde Graduate School, University of Science and Technology Beijing, Foshan 528399, China
* Correspondence: drzhangy@ustb.edu.cn
† These authors contributed equally to this work.

Abstract: The empirical parameters of mixing enthalpy (ΔH_mix), mixing entropy (ΔS_mix), atomic radius difference (δ), valence electron concentration (VEC), etc., are used in this study to design a depleted uranium high-entropy alloy (HEA). X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM) were used to assess the phase composition. Compression and hardness tests were conducted to select alloy constituents with outstanding mechanical properties. Based on the experimental results, the empirical criteria of HEAs are an effective means to develop depleted uranium high-entropy alloys (DUHEAs). Finally, we created UNb0.5Zr0.5Mo0.5 and UNb0.5Zr0.5Ti0.2Mo0.2 HEAs with outstanding all-round characteristics. Both alloys were composed of a single BCC structure. The hardness and strength of UNb0.5Zr0.5Mo0.5 and UNb0.5Zr0.5Ti0.2Mo0.2 were 305 HB and 1452 MPa, and 297 HB and 1157 MPa, respectively.

Keywords: depleted uranium high-entropy alloy; empirical parameters; BCC structure; phase composition; strengthen

1. Introduction

The concept of high-entropy alloys (HEAs) offers a new approach to exploring materials, expanding the research scope and the compositional palette. Due to the high entropy effect, HEAs can form a simple solid solution structure with excellent properties under a high concentration of multiple components [1]. HEAs with high strength and toughness [2,3], stability at high temperatures [4,5], and corrosion resistance [4,6] have been investigated. The HEA system mainly focuses on the 3rd to 5th period, 3d electron layer elements, and other main group elements, which usually form face-centered cubic (FCC) and body-centered-cubic (BCC) structures. Meanwhile, the rare earth elements, such as Tb, Dy, Lu, Tm, and Ho, usually form a hexagonal-close-packed (HCP) structure [7,8].

Unlike uranium, depleted uranium (DU) has very little radioactivity and is often used in military applications because of its self-sharpening properties and high density [9–11]. There are three structures of U (Table 1), and the γ-U structure with a BCC structure has ideal symmetry and properties at high temperatures. Alloying elements Zr [12], Ti [11,13], Mo [14], Nb [15,16], amongst others, usually have a wide range of solubility in γ-U of the BCC structure. Zr and Nb can dissolve completely with U and form the γ-phase at high temperatures. Ti can dissolve in the U matrix and form the δ-phase at a temperature above 725 °C, and the maximum solubility of Mo in γ-U is 21.2 weight percent (wt.%). HEAs

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have superior properties to traditional alloys. By applying the concept of high entropy to DU alloys and taking full advantage of γ-U, we can design DUHEAs with excellent performance and provide more options for high-performance structural materials.

Table 1. Uranium allotropes and their characteristics, data from [17,18].

| Allotrope | α-U | β-U | γ-U |
|-----------|-----|-----|-----|
| Temperature (°C) | <667.7 | 667.7~774.8 | 774.8~1132.3 |
| Crystal structure | ![Crystal Structure] | ![Crystal Structure] | ![Crystal Structure] |
| Density (g/cm³) | 19.05 | 18.13 | 17.91 |

2. Design Idea and Experimental Route for DUHEAs

2.1. Design Idea

HEAs design commonly includes high-throughput preparation, CALPHAD (phase diagram calculation) [19,20], and DFT (density functional theory) [21–23]. Generally, the factors considered in the calculation and simulation are ideal and are insufficient to reflect the actual casting process. In this study, we combined the solid solution formation criteria of HEA with an experimental search for high-performance DUHEAs. The elements Nb, Mo, Ti, and Zr, which have significant solubility in U, were selected. The physical properties are listed in Table 2.

Table 2. Physical properties of each element, data from [24–26].

| Element | U 238 | Nb | Zr | Ti | Mo |
|---------|-------|----|----|----|----|
| Atomic number | 92 | 41 | 40 | 22 | 42 |
| Atomic radius (pm) | 139 | 143 | 159 | 146 | 141 |
| Density (g/cm³) | 19.05 | 8.52 | 6.49 | 4.51 | 10.20 |
| Melting point (K) | 1405 | 2750 | 2128 | 1941 | 2896 |
| Electronegativity | 1.38 | 1.60 | 1.33 | 1.54 | 2.16 |
| Lattice content (pm) | 343.3 | 330.1 | 360.9 | 327.6 | 314.7 |
| Valence electron concentration (VEC) | 3 | 5 | 4 | 4 | 6 |

Yeh et al. [27] believe that the mixing entropy (ΔS_{mix}) is the main factor promoting the formation of solid solutions in HEAs. Zhang [28] extended the Hume-Rothery criterion to HEAs and proposed δ, ΔH_{mix}, and Ω as the factors affecting the formation of HEA solid solution phases.

The mixing entropy can be calculated by the following formula [1]:

\[ \Delta S_{mix} = -R \sum_{i=1}^{n} c_i \ln c_i \]  

(1)

where \( R \) is the ideal gas constant (J·mol⁻¹·K⁻¹); \( n \) is the number of components in the alloy; and \( c_i \) is the atomic fraction of the \( i \)th component in the alloy. From Formula (1), \( \Delta S_{mix} \) reaches the maximum when the atomic ratio of the elements in the alloy is equal. In general, alloys are assigned to the class of HEAs when the mixing entropy is higher than 1.5 \( R \) [29].

The parameter, δ, for the difference in atomic radius can be expressed as follows [1]:

\[ \delta = \sqrt{\sum_{i=1}^{n} c_i \left(1 - \frac{r_i}{R}\right)^2} \]  

(2)
\[ r = \sum_{i=1}^{n} c_i r_i \]

where \( r \) is the average atomic radius of the alloy (Å), and \( r_i \) is the atomic radius of the \( i \)th element of the alloy (Å).

The mixing enthalpy of a multi-component alloy can be calculated by the following formula [1]:

\[ \Delta H_{\text{mix}} = \sum_{i=1, j \neq i}^{n} 4H_{AB}^{\text{mix}} c_i c_j \]

where \( H_{AB}^{\text{mix}} \) is the mixing enthalpy of the \( i \)th and \( j \)th elements (kJ·mol\(^{-1}\)); \( c_i \) is the atomic percentage of the \( i \)th element in the alloy; and \( c_j \) is the atomic percentage of the \( j \)th elements in the alloy. The mixing enthalpy among U, Nb, Zr, Ti, and Mo are listed in Table 3.

| Element | U  | Nb | Zr | Ti | Mo |
|---------|----|----|----|----|----|
| Nb      | -  | 4  | -3 | 0  | 2  |
| Zr      | -  | -  | -  | -  | -  |
| Ti      | -  | -  | -  | -  | -  |
| Mo      | -  | -  | -  | -  | -  |

To simplify the prediction standard of an HEA solid solution structure, Zhang [30] proposed the \( \Omega \) parameter, the definition of which is expressed as follows [1]:

\[ \Omega = \frac{T_m \Delta S_{\text{mix}}}{|\Delta H_{\text{mix}}|} \]

where \( T_m \) is the melting point of a multi-component alloy (K); \( \Delta S_{\text{mix}} \) is the mixing entropy of a multi-component alloy (J·K\(^{-1}\)·mol\(^{-1}\)); and \( \Delta H_{\text{mix}} \) is the mixing enthalpy of a multi-component alloy (J·K\(^{-1}\)·mol\(^{-1}\)).

To develop DUHEAs with excellent mechanical properties, Zr and Nb, which can dissolve indefinitely with \( \gamma \)-U at a high temperature to form a BCC solid solution structure, were added to the DU ternary alloy. Then, Ti and Mo were added to the DU ternary alloy to refine its properties. The study path is shown in Figure 1.

![Figure 1. Alloy design path.](image)

2.2. Test Method

Ingots with a mass of approximately 50 g were prepared using a Vacuum arc melting furnace and pure metals of U, Nb, Mo, Ti, and Zr (purity was higher than 99 wt.\%). To ensure chemical homogeneity, the ingots were re-melted at least 4~5 times. An X-ray diffractometer (XRD, Bruker D8 Advance, Bruker AXS, Karlsruhe, Germany), with Cu K\(\alpha\) radiation, was used to measure the phase composition of the alloys. The scanning range was from 15\(^{\circ}\) to 90\(^{\circ}\), and the scanning speed was 5\(^{\circ}\)/min. The micro-morphologies of the alloys were observed by scanning electron microscopy (SEM, EVO18, Carl Zeiss AG, Jena, Germany) operating at 20 keV. The chemical composition was observed by energy-dispersive spectroscopy (EDS) equipped in the SEM. The standard bright-field (BF), image, and selected area electron diffraction (SAED) patterns were obtained by transmission electron microscope (TEM, Tecna F30, FEI, Hillsboro, OR, USA) operating at 300 kV, and the TEM data were processed using the Digital Micrograph software. Hardness
of the alloys was measured using the Wilson Brinell hardness meter BH3000 (Wilson, Norwood, MA, USA) under a load of 1840 N for 10 s. Room temperature compression tests were carried out by CMT5105 (Suns, Shenzhen, China). The specimen was a φ 6 mm cylinder with a height-to-diameter ratio of between 1.5 and 2. The compression tests were performed at a compression rate of $10^{-3}$ s$^{-1}$.

3. Design Process and Experimental Results

3.1. Ternary U-Nb-Zr Medium-Entropy Alloy (MEA)

Firstly, the U-Nb-Zr alloy system was studied. The thermodynamic parameters of the alloy system are listed in Table 4, and the relationship between δ-ΔH and δ-Ω of the alloy is shown in Figure 2. Zr and Nb are infinitely soluble in U, indicating that the alloy system has a strong tendency to form solid solutions. From Figure 2a all alloys had a disordered solid solution phase. While in Figure 2b, UNbZr0.5 and UNb1.5Zr are in the solid solution and intermetallic compound zones, UNbZr is on the boundary of the solid solution and intermetallic compound zones, which does not tend to form a solid solution. The value of VEC for every alloy was lower than 6.87, forming a stable BCC solid solution structure [31]. The results show that the alloys have a disordered solution phase.

Table 4. Thermodynamic parameters of the U-Nb-Zr alloy system.

| Alloys       | δ (%) | $\Delta H_{mix}$ (KJ/mol) | $\Delta S_{mix}$ (KJ/mol) | Tm (K) | Ω   | VEC |
|--------------|-------|---------------------------|---------------------------|--------|-----|-----|
| UNbZr        | 5.88  | 2.22                      | 9.13                      | 2094   | 8.6 | 4.00|
| UNb0.5Zr     | 6.26  | 0.64                      | 8.77                      | 1963   | 26.9| 3.80|
| UNbZr0.5     | 5.13  | 2.88                      | 8.77                      | 2087   | 6.4 | 4.00|
| UNb0.5Zr0.5  | 5.69  | 1.50                      | 8.64                      | 1922   | 11.1| 3.75|
| UNb1.5Zr     | 5.55  | 2.94                      | 8.97                      | 2188   | 6.7 | 4.14|
| UNbZr1.5     | 6.08  | 1.80                      | 8.97                      | 2099   | 10.5| 4.00|

Figure 2. The distribution of the entropy alloy in the ternary U-Nb-Zr in the relationship diagram of (a) δ-ΔH and (b) δ-Ω (SS: solid solution; IM: intermetallic compound).

The XRD pattern of the medium entropy alloys are presented in Figure 3. Regardless of the uranium oxides, the phase compositions of the alloys were almost identical and were composed of a single BCC phase. In addition, the diffraction peaks appeared to shift with the change in Nb and Zr contents. Combining Bragg’s Law with $d_{hk\\ell} = \frac{\delta}{\sqrt{h^2+k^2+l^2}}$ ($d_{hk\\ell}$ is the interplanar spacing), the diffraction peaks shifted suggesting lattice content changes [32]. Because U, Nb, and Zr have different lattice constants, the variation of the lattice constants of the alloys is complex. According to the electron diffraction of the UNbZr alloy in Figure 4a,b, the alloy exhibited a single-phase BCC structure, which is consistent with the prediction of the alloy formation.
Table 5. The hardness and strength of UNbZr with the change in Nb and Zr contents. Combining Bragg’s Law with the variation of the lattice constants of the alloys is complex. According to the electron diffraction patterns, the diffraction peaks shifted suggesting the lattice content changes [32]. Because U, Nb, and Zr have different lattice constants, the alloy compositions of UNb0.5Zr0.5 and UNb1.5Zr are uniform. The structure of the UNbZr alloy in Figure 4a,b, the alloy exhibited a single-phase BCC structure. In particular, the organization of UNb0.5Zr, UNbZr, and UNb1.5Zr were more homogeneous than that of UNb0.5Zr0.5 (see Figure 5). However, this study aimed to utilize waste DU and improve its potential availability; therefore, UNb0.5Zr0.5 was selected as the base alloy for the subsequent work.

The microstructures of the medium-entropy alloys in the U-Nb-Zr system are shown in Figure 5. The microstructure of UNbZr is presented in Figure 5a. The light-colored region was a U-enriched interdendritic structure, while Zr and Nb formed the BCC dendritic structure of the primary phase due to their higher melting points. When the Nb content decreased, as shown in Figure 5b, the segregation of UNb0.5Zr was more pronounced than that of UNbZr. When the Zr content decreased, the segregation of UNbZr0.5 decreased, as shown in Figure 5c, and the dendrite structure became finer. In Figure 5d,e, the alloy compositions of UNb0.5Zr0.5 and UNb1.5Zr are uniform. The structure of the UNbZr1.5 alloy is shown in Figure 5e, which was similar to UNbZr and displayed a typical as-cast dendrite structure (uniform region) with segregation of the components (U-enriched region).

The hardness and yield strength of the alloys of the U-Nb-Zr system are given in Table 5. The hardness and strength of UNbZr0.5 and UNbZr1.5 were lower than those of other alloys. It seems that the mechanical properties of UNb0.5Zr, UNbZr, and UNb1.5Zr were higher than those of UNb0.5Zr0.5. In particular, the organization of UNb0.5Zr was more homogeneous than that of UNb0.5Zr0.5 (see Figure 5). However, this study aimed to utilize waste DU and improve its potential availability; therefore, UNb0.5Zr0.5 was selected as the base alloy for the subsequent work.

Figure 3. XRD diffraction patterns of the medium entropy alloy in U-Nb-Zr.

Figure 4. (a) TEM bright-field image; (b) selected area-electron-diffraction image of the UNbZr alloy.

Figure 5. The microstructure of UNbZr is presented in Figure 5a. The light-colored region was a U-enriched interdendritic structure, while Zr and Nb formed the BCC dendritic structure of the primary phase due to their higher melting points. When the Nb content decreased, as shown in Figure 5b, the segregation of UNb0.5Zr was more pronounced than that of UNbZr. When the Zr content decreased, the segregation of UNbZr0.5 decreased, as shown in Figure 5c, and the dendrite structure became finer. In Figure 5d,e, the alloy compositions of UNb0.5Zr0.5 and UNb1.5Zr are uniform. The structure of the UNbZr1.5 alloy is shown in Figure 5e, which was similar to UNbZr and displayed a typical as-cast dendrite structure (uniform region) with segregation of the components (U-enriched region).
With the addition of Ti and Mo, the lattice constant of the matrix decreased, indicating the

drop 

Thermodynamic parameters of UNb0.5Zr0.5-X (Ti/Mo) HEAs. From the relationship
diagram of δ-AH and δ-Ω in Figure 6, the studied UNb0.5Zr0.5-X (Ti/Mo) HEAs were solid
solution phases. Based on their VEC, it was discovered that these alloys were BCC phases.

Table 6. Thermodynamic parameters of UNb0.5Zr0.5-X HEAs.

| Alloys         | δ (%) | ΔHmix (KJ/mol) | ΔSmix (KJ/mol) | Tm (K) | Ω  | VEC  |
|----------------|-------|----------------|----------------|--------|----|------|
| UNb0.5Zr0.5Ti0.2 | 5.42  | 1.40           | 10.39          | 1924   | 14.3| 3.77 |
| UNb0.5Zr0.5Ti0.5 | 5.09  | 1.28           | 11.07          | 1926   | 16.7| 3.80 |
| UNb0.5Zr0.5Ti   | 4.64  | 1.11           | 11.05          | 1928   | 19.2| 3.83 |
| UNb0.5Zr0.5Mo0.2| 5.49  | 0.58           | 10.39          | 2011   | 36.1| 3.95 |
| UNb0.5Zr0.5Mo0.5| 5.23  | -0.32          | 11.07          | 2117   | 73.3| 4.20 |
| UNb0.5Zr0.5Mo   | 4.87  | -1.11          | 11.05          | 2247   | 22.4| 4.50 |

The XRD results of UNb0.5Zr0.5-X (Ti/Mo) HEAs presenting BCC structures are repre-
sented in Figure 7. Ignoring the uranium oxides, most of the alloys consisted of a single
BCC structure, UNb0.5Zr0.5Ti and UNb0.5Zr0.5Mo HEAs forming two BCC structures. The
diffraction peak changed to a higher angle as the concentrations of Ti and Mo grew, show-
ing that the lattice constant dropped [32]. As presented in Table 2, the lattice contents of U,
Mo, and Ti at room temperature are 343.3 pm, 314.7 pm, and 327.6 pm [17,26], respectively.
With the addition of Ti and Mo, the lattice constant of the matrix decreased, indicating the
occurrence of solid solution and the generation of lattice distortion. When the content of Mo reached the maximum, UNb0.5Zr0.5Mo was composed of two BCC structures, which was because Mo has the highest melting point of the elements.

Figure 6. (a) δ-ΔH and (b) δ-Ω distribution diagram of UNb0.5Zr0.5-X HEAs.

Figure 7. XRD pattern of the UNb0.5Zr0.5-X (Ti/Mo) HEAs.

The as-cast microstructures of UNb0.5Zr0.5-X (Ti/Mo) HEAs are shown in Figure 8, and the alloys all have a typical as-cast dendritic structure similar to the U-Nb-Zr system alloys. Composition segregation was obvious as the concentration of Ti and Mo increased. UNb0.5Zr0.5Ti0.2, UNb0.5Zr0.5Ti0.5, UNb0.5Zr0.5Ti, and UNb0.5Zr0.5Mo0.2, and UNb0.5Zr0.5Mo0.5 consisted of a uniform region, a U-enriched region and a UOx region. Compared with UNb0.5Zr0.5Ti0.2 and UNb0.5Zr0.5Ti0.5, the segregation of the U-enriched region in UNb0.5Zr0.5Ti was high obviously. UNb0.5Zr0.5Mo was composed of a U-enriched region, Mo-enriched region, and UOx, which was different from UNb0.5Zr0.5Mo0.2 and UNb0.5Zr0.5Mo0.5. As Figure 8f shows, the Mo-enriched region formed the BCC2 phase that is in line with the XRD patterns of Figure 7.

Table 7 shows the Brinell hardness and yield strength of the UNb0.5Zr0.5-X HEAs. The addition of Ti significantly reduced the hardness of the alloy. When the molar ratio of Ti was 0.5, the yield strength of the alloy reached 881 MPa. While the hardness of the alloy improved dramatically as the Mo percentage increased, the yield strength decreased. This was because the hardness of Mo was higher than that of other elements. In addition, the melting point of Mo was the highest of the five elements, which will improve segregation during the solidification process. As a result, the hardness increased dramatically, and segregation of the alloy increased along with the Mo content, dramatically influencing the mechanical characteristics of the alloy.
Table 7. Hardness and strength of the UNb\(_{0.5}\)Zr\(_{0.5}\)-X HEAs.

| Properties          | UNb\(_{0.5}\)Zr\(_{0.5}\)Ti\(_{0.2}\) | UNb\(_{0.5}\)Zr\(_{0.5}\)Ti\(_{0.5}\) | UNb\(_{0.5}\)Zr\(_{0.5}\)Ti | UNb\(_{0.5}\)Zr\(_{0.5}\)Mo\(_{0.2}\) | UNb\(_{0.5}\)Zr\(_{0.5}\)Mo\(_{0.5}\) | UNb\(_{0.5}\)Zr\(_{0.5}\)Mo |
|---------------------|--------------------------------------|--------------------------------------|-------------------------------|----------------------------------|----------------------------------|---------------------------|
| Hardness (HB)       | 233                                  | 220                                  | 214                           | 289                             | 305                             | 367                       |
| Strength (MPa)      | 760                                  | 881                                  | 754                           | /                               | 1452                            | 1668.9 (Crashed)           |

3.3. Quinary U-Nb-Zr-Ti-Mo HEAs

We can observe from the previous section on the quaternary HEAs that the proposed alloys could form a stable solid solution phase of a BCC structure. The UNb\(_{0.5}\)Zr\(_{0.5}\)Ti\(_{0.2}\), UNb\(_{0.5}\)Zr\(_{0.5}\)Ti\(_{0.5}\), UNb\(_{0.5}\)Zr\(_{0.5}\)Mo\(_{0.2}\), and UNb\(_{0.5}\)Zr\(_{0.5}\)Mo\(_{0.5}\) alloys had the most uniform elemental distributions, and the segregation phenomenon was not observed. A five-element DUHEA was prepared by varying the ratio of Ti and Mo and choosing UNb\(_{0.5}\)Zr\(_{0.5}\)Ti\(_{x}\)Mo\(_x\).

The thermodynamic properties of Nb-Zr-U-Ti-Mo HEAs were all solid solution phases, as evidenced by the relationship between $\delta$-$\Delta H$ and $\delta$-$\Omega$ in Figure 9. Based on its VEC, we can predict that the developed alloy will be a BCC phase.

Table 8. Thermodynamic parameters of U-Nb-Zr-Ti-Mo HEAs.

| Alloys              | $\delta$ (%) | $\Delta H_{mix}$ (KJ/mol) | $\Delta S_{mix}$ (KJ/mol) | $T_m$ (K) | $\Omega$ | VEC |
|---------------------|--------------|---------------------------|---------------------------|-----------|----------|-----|
| UNb\(_{0.5}\)Zr\(_{0.5}\)Ti\(_{0.2}\)Mo\(_{0.2}\) | 5.26         | 0.51                      | 11.91                     | 2005      | 46.46    | 3.96 |
| UNb\(_{0.5}\)Zr\(_{0.5}\)Ti\(_{0.5}\)Mo\(_{0.5}\) | 4.79         | -0.44                     | 12.98                     | 2088      | 60.94    | 4.17 |
The phase composition and microstructure of the five-element DUHEA were investigated. Figure 10 shows the XRD data on the UNb$_{0.5}$Zr$_{0.5}$Ti$_x$Mo$_{0.5}$ (x = 0.2, 0.5) HEA. UNb$_{0.5}$Zr$_{0.5}$Ti$_{0.2}$Mo$_{0.2}$ was composed of a single BCC structure and UNb$_{0.5}$Zr$_{0.5}$Ti$_{0.5}$Mo$_{0.5}$ formed two BCC structures. The addition of Ti and Mo contributed to the formation of BCC2. In addition, when the concentration of Ti and Mo increased, the diffraction peaks were shifted to higher angles, indicating a decrease in the lattice constants. Moreover, the diffraction peaks became broader with the increase in the Ti and Mo contents, indicating grain refinement [33].

The as-cast structures of the UNb$_{0.5}$Zr$_{0.5}$Ti$_{0.2}$Mo$_{0.2}$ and UNb$_{0.5}$Zr$_{0.5}$Ti$_{0.5}$Mo$_{0.5}$ alloys are shown in Figure 11. These alloys had a typical cast dendritic structure of a uniform composition region and U-enriched region between the dendritic structures. It can be observed that the structure segregation phenomenon of the alloys improved as Ti and Mo concentrations increased. This was due to the fact that Mo had a high melting point (higher than U’s melting point) and element redistribution during solidification. The alloy components are equally distributed without noticeable segregation, as seen in the surface scan findings of UNb$_{0.5}$Zr$_{0.5}$Ti$_{0.2}$Mo$_{0.2}$ in Figure 12.

The Brinell hardness and yield strength of the UNb$_{0.5}$Zr$_{0.5}$Ti$_x$Mo$_x$ HEAs are listed in Table 9. The addition of Ti and Mo promoted the hardness and yield strength of the alloys, and plasticity reduced dramatically. The mixing enthalpy of Mo with Nb, Zr, and Ti was negative, and Mo had a higher melting point, resulting in component segregation. It can be demonstrated by examining UNb$_{0.5}$Zr$_{0.5}$Ti$_{0.5}$Mo$_{0.5}$, which has a higher hardness of 350 HB than that of UNb$_{0.5}$Zr$_{0.5}$Ti$_{0.2}$Mo$_{0.2}$.
The as-cast structures of the UNb$_{0.5}$Zr$_{0.5}$Ti$_{0.2}$Mo$_{0.2}$ and UNb$_{0.5}$Zr$_{0.5}$Ti$_{0.5}$Mo$_{0.5}$ alloys are BCC solid solution structures, per the solid-solution formation criteria and microstructure characterization. Figure 13 shows the solid-solution formation criteria and microstructure characterization. Figure 13 shows findings of UNb$_{0.5}$Zr$_{0.5}$Ti$_{0.2}$Mo$_{0.2}$ in Figure 12.

Microstructures of the (a) UNb$_{0.5}$Zr$_{0.5}$Ti$_{0.2}$Mo$_{0.2}$ and (b) UNb$_{0.5}$Zr$_{0.5}$Ti$_{0.5}$Mo$_{0.5}$ alloys.

EDS map of the UNb$_{0.5}$Zr$_{0.5}$Ti$_{0.2}$Mo$_{0.2}$ alloy.

**Table 9.** Hardness and strength of the UNb$_{0.5}$Zr$_{0.5}$Ti$_{x}$Mo$_{y}$ HEAs.

| Properties       | UNb$_{0.5}$Zr$_{0.5}$Ti$_{0.2}$Mo$_{0.2}$ | UNb$_{0.5}$Zr$_{0.5}$Ti$_{0.5}$Mo$_{0.5}$ |
|------------------|------------------------------------------|------------------------------------------|
| Hardness (HB)    | 297                                      | 350                                      |
| Strength (MPa)   | 1157                                     | 1215 (Crashed)                           |

4. Discussion

The researched alloys in the present article are all BCC solid solution structures, per the solid-solution formation criteria and microstructure characterization. Figure 13 shows the concept of the DUHEA design process, which begins with the ternary U-Nb-Zr system, adds Ti and Mo elements to create the quaternary alloys and, ultimately, finishes with the quinary UNb$_{0.5}$Zr$_{0.5}$Ti$_{x}$Mo$_{y}$ alloy. The mixing enthalpy of U with Nb, Ti, Zr, and Mo had a significant impact on the structure and mechanical properties of the studied alloys. The relationship between the mixing enthalpy and the mechanical characteristics of the alloys are presented in Figure 14. The compressive yield strength and hardness exhibited a rising trend as the mixing enthalpy fell. Though UNb$_{0.5}$Zr$_{0.5}$Ti$_{0.5}$Mo$_{0.5}$ and UNb$_{0.5}$Zr$_{0.5}$Mo$_{0.5}$ had higher strength, severe component segregation microstructures resulted in poor plasticity. This was due to the melting point of Mo being higher than those of other elements, resulting in component segregation and poor performance. Finally, based on our combined theoretical and experimental results, UNb$_{0.5}$Zr$_{0.5}$Mo$_{0.5}$ and UNb$_{0.5}$Zr$_{0.5}$Ti$_{0.2}$Mo$_{0.2}$ had a homogeneous structure and outstanding mechanical characteristics.
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5. Conclusions

In this paper, we examined the composition of UNb0.5Zr0.5Mo0.5 and UNb0.5Zr0.5Ti0.2Mo0.2, finding both to possess a homogeneous structure, low segregation, and outstanding mechanical properties. The alloys examined were screened during the design process from the DU ternary alloy to DUHEA according to the formation law of HEAs and based on experimental results. UNb0.5Zr0.5Mo0.5 and UNb0.5Zr0.5Ti0.2Mo0.2 were composed of a single BCC structure, which was in line with our theoretical calculations. The hardness and strength of UNb0.5Zr0.5Mo0.5 and UNb0.5Zr0.5Ti0.2Mo0.2 were 305 HB and 1452 MPa, and 297 HB and 1157 MPa, respectively. This suggests that the HEA phase-formation criteria could have a wide range of applications in the design of DUHEAs, providing promising theoretical direction for the future development of specific BCC-structured HEAs.

Figure 13. Design process of a DUHEA.

Figure 14. Trend graph of the relationship between the mixed enthalpy and mechanical properties of the U-Nb-Zr-Ti-Mo HEAs.
Data Availability Statement: All data included in this study are available from the corresponding author on reasonable request.

Conflicts of Interest: The authors declare no conflict of interest.

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