A simple approach to model the yield strength of body centered cubic solid solution refractory high entropy alloys

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Abstract

A simple fitting approach is used for modeling the compressive yield strength of body centered cubic (bcc) solid solution high entropy alloys in Al-Hf-Nb-Mo-Ta-Ti-V-Zr system. It is proposed that the yield strength could be modeled by a polynomial where the experimental data can be used for finding the polynomial’s coefficients. The results show that the proposed polynomial could model the yield strength of solid solution alloys relatively well. The developed polynomial is used for predicting the strength of RHEAs in Hf-Mo-Nb-Ta-Ti-V-Zr system. It is observed that the yield strength of alloys within this system increases with the additions of Mo and Zr and decreases with the addition of Ti. Furthermore, the model predicts that the yield strength increases with increasing the value of parameters valence electron concentration (VEC) and atomic size difference (ASD). Although the developed polynomial does not consider the mechanisms involved in the strengthening of alloys, it can be considered as a straightforward method for assessing the strength of solid solution RHEAs.
1. Introduction

High entropy alloys (HEAs) or multi-principal-element alloys are a new group of metallic alloys with encouraging functional and mechanical properties [1-4]. The main difference between HEAs and traditional alloys is that HEAs contain multiple principal elements while traditional alloys are usually based on one dominant element [1-4]. HEAs which are based on refractory elements such as Hf, Nb, Mo, Ta, W, V and Zr are called refractory high entropy alloys (RHEAs) after Senkov et al. [5-6]. RHEAs have shown very promising high-temperature mechanical properties and are being considered as “future materials for high-temperature structural applications beyond Ni-based superalloys” [5]. A detailed review regarding the microstructure and properties of RHEAs can be found in [5].

The final goal of many research works in the field of HEAs is to identify alloys with desired properties. However, because HEAs contain several principal elements, a great number of alloys need to be examined in this regard. Examination a great number of alloys is not possible in practice. Therefore, it is very important to develop convenient methods and models which can predict the microstructure and properties of HEAs. In this regard, several research works have focused on developing models for predicting the microstructure or mechanical properties of HEAs [1-5]. Although these approaches have been successfully applied, they have their own limitations. The objective of the present work is to introduce a new methodology (data-based modeling and fitting) for predicting the properties of HEAs. In the present work, the approach is applied for predicting the yield strength of body centered cubic (bcc) solid solution RHEAs in Al-Hf-Nb-Mo-Ta-Ti-V-Zr system. Although the introduced approach (data-based modeling and fitting)
do not explain the mechanisms involved in the strengthening of alloys, it can be considered as a straightforward method for assessing the strength of solid solution RHEAs in Al-Hf-Nb-Mo-Ta-Ti-V-Zr system. Therefore, the proposed approach can be considered as a valuable tool for designing RHEAs in this alloy system.

2. Methodology

2.1. Experimental data

RHEAs (more than 80 alloys) which are shown in Table 1 are used in the preset work. The data in Table 1 are gathered from references [7-37]. All of the alloys in Table 1 were made by vacuum arc melting technique, and a single phase bcc solid solution microstructure was reported for all of them in the as-cast condition. Some Ti rich alloys are also listed in Table 1. These Ti rich alloys are being considered as promising candidates for biomedical applications [35-37]. The compressive yield stress for each alloy in the as-cast condition is shown the last column. It can be seen that the dataset in Table 1 covers a relatively broad range of chemical compositions including Ti and Nb rich alloys. The composition domain which is covered by alloys in Table 1 is schematically shown in Figure 1. In addition to the experimental data in Table 1, following estimations [27, 38] are also used for the yield strength of bcc elements and binary systems: $\sigma_{Mo} = 450$ MPa [27], $\sigma_{Nb} = 250$ MPa [27], $\sigma_{Ta} = 350$ [27], $\sigma_{V} = 300$ MPa [27], $\sigma_{NbTa} = 320$ MPa [27, 38], $\sigma_{MoTa} = 1200$ MPa [27, 39], and $\sigma_{VNb} = 800$ MPa [40].
Figure 1. The composition domain which is covered by alloys in Table 1 containing Ti and Nb rich alloys
Table 1. Chemical compositions of investigated alloys and the compressive yield stress (S) for each alloy in the as-cast condition; all of the alloys have a single phase bcc solid solution microstructure in the as-cast condition

| Alloy | S(MPa) | Al | Hf | Mo | Nb | Ta | Ti | V | Zr |
|-------|--------|----|----|----|----|----|----|---|----|
| HfNbTaTiZr [7] | 1073 | 0 | 20 | 0 | 20 | 20 | 20 | 0 | 20 |
| A10.3HfNbTaTiZr [7] | 1188 | 5.5 | 19 | 0 | 18.9 | 18.9 | 18.9 | 0 | 18.9 |
| A10.5HfNbTaTiZr [7] | 1302 | 9.1 | 18 | 0 | 18.2 | 18.18 | 18.2 | 0 | 18.2 |
| A10.75HfNbTaTiZr [7] | 1415 | 13 | 17 | 0 | 17.4 | 17.4 | 17.4 | 0 | 17.4 |
| HfMo0.1NbTaTiZr [8] | 1015 | 0 | 20 | 0 | 20 | 20 | 20 | 0 | 20 |
| HfMo0.25NbTaTiZr [8] | 1112 | 0 | 19 | 4.8 | 19.1 | 19.05 | 19.1 | 0 | 19.1 |
| HfMo0.5NbTaTiZr [8] | 1317 | 0 | 18 | 9.1 | 18.2 | 18.18 | 18.2 | 0 | 18.2 |
| HfMo0.75NbTaTiZr [8] | 1373 | 0 | 17 | 13 | 17.4 | 17.39 | 17.4 | 0 | 17.4 |
| HfMoNbTaTiZr [8] | 1512 | 0 | 17 | 17 | 16.7 | 16.67 | 16.7 | 0 | 16.7 |
| HfNbTiZr [9] | 879 | 0 | 25 | 0 | 25 | 0 | 25 | 0 | 25 |
| TiHfZrTaNb [10] | 905 | 0 | 20 | 0 | 20 | 20 | 20 | 0 | 20 |
| Hf0.5Nb0.5Ta0.5Ti1.5Zr [11] | 903 | 0 | 13 | 0 | 12.5 | 12.5 | 37.5 | 0 | 25 |
| AlNbTaTi [12] | 1150 | 25 | 0 | 0 | 25 | 25 | 25 | 0 | 0 |
| HfMoTaTiZr [13] | 1600 | 0 | 20 | 20 | 0 | 20 | 20 | 0 | 20 |
| HfMoNbTaTiZr [13] | 1512 | 0 | 17 | 17 | 16.7 | 16.67 | 16.7 | 0 | 16.7 |
| NbMoTiWfHf [14] | 521 | 0 | 0 | 12 | 70 | 0 | 18.1 | 0 | 0 |
| NbMoTiWfHf [14] | 719 | 0 | 0 | 14 | 67.8 | 0 | 18.1 | 0 | 0 |
| NbMoTiWfHf [14] | 780 | 0 | 0 | 33 | 34.7 | 0 | 28.5 | 0 | 0 |
| NbMoTiWfHf [14] | 1100 | 0 | 0 | 25 | 25 | 0 | 25 | 0 | 25 |
| Hf0.4Nb1.5Ti1.55Ta1.55Zr0.64 [15] | 822 | 0 | 8 | 0 | 30.8 | 30.8 | 17.7 | 0 | 12.7 |
| Hf0.5Mo0.5NbTiZr [16] | 1176 | 0 | 13 | 13 | 25 | 0 | 25 | 0 | 25 |
| HfMoNbTiZr [17] | 1719 | 0 | 20 | 20 | 20 | 0 | 20 | 0 | 20 |
| HfNbTaZr [18] | 1315 | 0 | 25 | 0 | 25 | 25 | 0 | 0 | 25 |
| MoNbTiZr [19] | 1560 | 0 | 0 | 25 | 25 | 0 | 25 | 0 | 25 |
| TiZrNbMoV0.25 [19] | 1750 | 0 | 0 | 23.53 | 23.53 | 0 | 23.53 | 5.88 | 23.53 |
| HfMoTaTiZr [20] | 1600 | 0 | 20 | 20 | 0 | 20 | 20 | 0 | 20 |
| HfMoNbTiZr [20] | 1351 | 0 | 20 | 20 | 20 | 0 | 20 | 0 | 20 |
| HfMoNbTaZr [20] | 1524 | 0 | 20 | 20 | 20 | 0 | 20 | 0 | 20 |
| HfMoNbTaTi [20] | 1367 | 0 | 20 | 20 | 20 | 20 | 0 | 0 | 0 |
| HfNb0.5Mo0.5TiZr [21] | 1195 | 0 | 25 | 13 | 12.5 | 0 | 25 | 0 | 25 |
| HfNb0.5Ta0.5ZrTi [21] | 738 | 0 | 25 | 0 | 12.5 | 12.5 | 25 | 0 | 25 |
| Mo1.4Nb1.4Ta1.4Ti0.6Zr0.6 [22] | 1275 | 0 | 0 | 26 | 25.9 | 25.93 | 11.1 | 0 | 11.1 |
| Mo0.6Nb0.6Ta0.6Ti1.4Zr1.4 [22] | 1160 | 0 | 0 | 13 | 13.1 | 13.05 | 30.4 | 0 | 30.4 |
| Mo0.5NbTaTi1.5Zr [22] | 1050 | 0 | 0 | 10 | 20 | 20 | 30 | 0 | 20 |
| Mo0.3NbTaTi1.7Zr [22] | 1025 | 0 | 0 | 6 | 20 | 20 | 34 | 0 | 20 |
| Ti50-xAlxV20Nb20Mo10 [23] | 900 | 10 | 0 | 10 | 20 | 0 | 40 | 20 | 0 |
| Ti50-xAlxV20Nb20Mo10 [23] | 971 | 15 | 0 | 10 | 20 | 0 | 35 | 20 | 0 |
| Composition | Samples | 20 | 0 | 10 | 20 | 0 | 30 | 20 | 0 |
|-------------|---------|----|---|----|---|---|----|---|---|
| Ti<sub>50</sub>-Al<sub>1.67</sub>Mo<sub>20</sub>Nb<sub>20</sub>Mo<sub>10</sub> [23] | 1187 | 20 | 0 | 10 | 20 | 0 | 30 | 20 | 0 |
| MoNbTiV [24] | 1200 | 0 | 0 | 25 | 25 | 0 | 25 | 25 | 0 |
| Al<sub>0.25</sub>MoNbTiV [24] | 1250 | 5.88 | 0 | 23.53 | 23.53 | 0 | 23.53 | 23.53 | 0 |
| Al<sub>0.5</sub>MoNbTiV [24] | 1625 | 11.12 | 0 | 22.22 | 22.22 | 0 | 22.22 | 22.22 | 0 |
| Al<sub>0.75</sub>MoNbTiV [24] | 1260 | 15.8 | 0 | 21.05 | 21.05 | 0 | 21.05 | 21.05 | 0 |
| AlMoNbTiV [24] | 1375 | 20 | 0 | 20 | 20 | 0 | 20 | 20 | 0 |
| MoVTaTi [25] | 1221 | 0 | 0 | 25 | 25 | 0 | 25 | 25 | 0 |
| HfMo<sub>0.5</sub>NbTiV<sub>0.5</sub> [26] | 1260 | 0 | 25 | 12.5 | 25 | 0 | 25 | 12.5 | 0 |
| Mo<sub>0.1</sub>NbTiV<sub>0.3</sub>Zr [26] | 932 | 0 | 0 | 2.94 | 29.41 | 0 | 29.41 | 8.83 | 29.41 |
| Mo<sub>0.3</sub>NbTiV<sub>0.3</sub>Zr [26] | 1312 | 0 | 0 | 8.33 | 27.78 | 0 | 27.78 | 8.33 | 27.78 |
| Mo<sub>0.5</sub>NbTiV<sub>0.3</sub>Zr [26] | 1289 | 0 | 0 | 6.96 | 23.26 | 0 | 23.26 | 23.26 | 23.26 |
| Mo<sub>0.7</sub>NbTiV<sub>0.5</sub>Zr [26] | 1436 | 0 | 0 | 17.5 | 25 | 0 | 25 | 7.5 | 25 |
| Mo<sub>0.9</sub>NbTiV<sub>0.5</sub>Zr [26] | 1706 | 0 | 0 | 14.88 | 21.28 | 0 | 21.28 | 21.28 | 21.28 |
| Mo<sub>1.3</sub>NbTiV<sub>0.5</sub>Zr [26] | 1603 | 0 | 0 | 28.26 | 21.74 | 0 | 21.74 | 6.52 | 21.74 |
| Mo<sub>1.3</sub>NbTiV<sub>0.5</sub>Zr [26] | 1496 | 0 | 0 | 24.52 | 18.87 | 0 | 18.87 | 18.87 | 18.87 |
| Mo<sub>0.5</sub>NbTaV<sub>0.5</sub>Zr [26] | 1576 | 0 | 0 | 31.26 | 20.83 | 0 | 20.83 | 6.25 | 20.83 |
| TiZrNbV [26] | 1104 | 0 | 0 | 0 | 25 | 0 | 25 | 25 | 25 |
| TiZrNbV<sub>0.5</sub>Mo [26] | 866 | 0 | 0 | 0 | 30.3 | 0 | 30.3 | 9.1 | 30.3 |
| TiZrNbVMo [26] | 1779 | 0 | 0 | 20 | 20 | 0 | 20 | 20 | 20 |
| MoNbTiV<sub>0.5</sub>Zr [26] | 1455 | 0 | 0 | 23.25 | 23.25 | 0 | 23.25 | 7 | 23.25 |
| MoNbTaTiV [27] | 1400 | 0 | 0 | 20 | 20 | 20 | 20 | 20 | 0 |
| MoNbTaV [28] | 1500 | 0 | 0 | 25 | 25 | 25 | 0 | 25 | 0 |
| NbTaV [29] | 965 | 0 | 0 | 0 | 25 | 25 | 25 | 0 | 25 |
| TiZrHf<sub>0.5</sub>Nb<sub>0.25</sub> [30] | 1115 | 0 | 10.53 | 0 | 5.26 | 0 | 42.11 | 21.05 | 21.05 |
| Ti<sub>2</sub>ZrHf<sub>2</sub>Nb<sub>0.5</sub> [30] | 1065 | 0 | 10 | 0 | 10 | 0 | 40 | 20 | 20 |
| Ti<sub>2</sub>ZrHf<sub>0.5</sub>Nb<sub>0.75</sub> [30] | 1025 | 0 | 9.5 | 0 | 14.3 | 0 | 38.2 | 19 | 19 |
| Ti<sub>2</sub>ZrHf<sub>0.5</sub>Nb [30] | 980 | 0 | 16.67 | 0 | 16.67 | 0 | 33.34 | 16.67 | 16.65 |
| TaZrNbTi [31] | 1100 | 0 | 0 | 0 | 25 | 25 | 25 | 0 | 25 |
| TiZrNbHf [32] | 1000 | 0 | 25 | 0 | 25 | 0 | 25 | 0 | 25 |
| NbMoTa [33] | 999 | 0 | 0 | 33 | 34 | 33 | 0 | 0 | 0 |
| TiZrNbTa [34] | 925 | 0 | 0 | 0 | 25 | 25 | 25 | 0 | 25 |
| Ti<sub>3</sub>Zr<sub>1.67</sub>Nb<sub>1.67</sub>Ta<sub>5</sub> [34] | 1075 | 0 | 0 | 0 | 31.66 | 5 | 31.67 | 0 | 31.67 |
| Ti<sub>3</sub>Zr<sub>3</sub>Nb<sub>25</sub>Ta<sub>5</sub> [34] | 1000 | 0 | 0 | 0 | 25 | 5 | 35 | 0 | 35 |
| Ti<sub>4</sub>Zr<sub>45</sub>Nb<sub>5</sub>Ta<sub>5</sub> [34] | 850 | 0 | 0 | 0 | 5 | 5 | 45 | 0 | 45 |
| Ti<sub>21.67</sub>Zr<sub>21.67</sub>Nb<sub>21.66</sub>Ta<sub>35</sub> [34] | 1250 | 0 | 0 | 0 | 21.66 | 35 | 21.67 | 0 | 21.67 |
| Ti<sub>15</sub>Zr<sub>15</sub>Nb<sub>35</sub>Ta<sub>35</sub> [34] | 1050 | 0 | 0 | 0 | 35 | 35 | 35 | 15 | 0 |
| Ti-Nb-Zr [35] | 720 | 0 | 0 | 0 | 25 | 0 | 57 | 0 | 18 |
| Ti-Nb-Zr [35] | 750 | 0 | 0 | 0 | 22 | 0 | 54 | 0 | 24 |
| Ti-Nb-Zr [35] | 740 | 0 | 0 | 0 | 21 | 0 | 52 | 0 | 27 |
| Ti-Nb-Zr [35] | 715 | 0 | 0 | 0 | 19 | 0 | 50 | 0 | 31 |
2.2. Proposed methodology

First the strength of binary solid solution refractory alloys can be considered. Figure 2 shows the critical resolved shear stress (\(\tau_{CRSS}\)) of Nb-Ta alloy single crystals at room temperature [38]. It can be seen that the strength of Nb-Ta bcc solid solution alloys can be modeled by a polynomial where the polynomial equation can be written as following

\[
\tau_{CRSS} = 0.8787 \times Nb - 0.0062 \times Nb^2 + 0.0042 \times Ta^2
\]

where \(Nb\) and \(Ta\) show the atomic concentrations of niobium and tantalum in atomic percent. Therefore, the solid solution strengthening can be modeled by a polynomial equation. As other examples, solid solution strengthening in Mo-Ta [39], Mo-W [39] and V-Nb [40] alloys can be considered. Figure 3 shows the hardness values of Mo-Ta and Mo-W solid solution bcc alloys in homogenized states [39]. It can be observed that the strength of solid solution alloys can be modeled by polynomials as following

\[
H_{Mo-Ta} = 15.0133 \times Mo - 0.1335 \times Mo^2 + 0.0108 \times Ta^2
\]

\[
H_{Mo-W} = 4.795 \times W + 0.017 \times Mo^2 - 0.0082 \times W^2
\]

where \(Mo\), \(Ta\) and \(W\) show the atomic concentration of molybdenum, tantalum and tungsten respectively.
Figure 2. Experimental data for the critical resolved shear stress ($\tau_{\text{CRSS}}$) of Nb-Ta alloy single crystals at room temperature [38] and the proposed polynomial for modeling the strength (see the text for the equation of polynomial).

Figure 3. Experimental data for the hardness ($H$) of (a) Mo-Ta and (b) Mo-W solid solution bcc alloys at room temperature [39] and the proposed polynomials for modeling the hardness (see the text for the equations of polynomials).
According to the results in Figures 2 and 3, it may be assumed that the strength of solid solution bcc RHEAs can also be modeled by a polynomial. Therefore, the following polynomial is proposed in the present work for modeling the compressive yield stress ($S$) of alloys listed in Table 1

$$S = \sum_{i=1}^{8} (a_i C_i + b_i C_i^2)$$

where $a_i$ and $b_i$ are coefficients to be determined and $C_i$ is the atomic concentration (at. %) of element $i$. For obtaining the coefficients $a_i$ and $b_i$, the above equation is fitted to the experimental dataset in Table 1, and the obtained values for coefficients are shown in Table 2.

Table 2. The values of coefficients obtained after fitting the proposed polynomial to the experimental dataset in Table 1

| constant | Al  | Hf   | Mo   | Nb   | Ta   | Ti   | V    | Zr   |
|----------|-----|------|------|------|------|------|------|------|
| $a_i$    | 15.828 | 17.104 | 36.464 | 7.242 | 10.725 | -0.517 | 19.312 | 34.581 |
| $b_i$    | 0.317 | -0.286 | -0.324 | -0.05 | -0.079 | 0.062 | -0.163 | -0.474 |

The comparison between the predictions and experimental results is shown in Figure 4. Considering the errors and deviations which exist for the yield stress values in Table 1, it can be seen that a relatively good agreement exists between predictions and experimental results. Therefore, one can concluded that the proposed polynomial can be used for modeling the compressive yield stress of bcc solid solution alloys in Al-Hf-Nb-Mo-Ta-Ti-V-Zr system. An important point regarding the developed polynomial is that it only needs element concentrations
as inputs and no mechanical or structural constants are needed; therefore, it can be applied easily for predicting the strength of RHEAs.

![Graph](image)

**Figure 4.** Comparison between the predictions and experimental results for the compressive yield stress ($S$) of alloys in Table 1

### 3. Results and discussions

For verifying the extrapolating ability of developed polynomial, the polynomial is used for predicting the strength of RHEAs in Table 3. A single phase bcc solid solution microstructure in the as-cast condition is reported for all of alloys in Table 3 [35-39]. Because strength values in Table 3 were obtained via tensile or microhardness tests, inconsistencies may be expected between the predictions and experimental results. Furthermore, the Hf and V content of ternary alloys in Table 3 are out of the composition domain in Figure 1. Therefore, the developed polynomial cannot be used for these alloys, and the predictions results may not be accurate. Nevertheless, the polynomial is applied for these alloys as well.
Table 3. Experimental data (as-cast condition) used for evaluating the extrapolating ability of developed polynomial

| Alloy                  | as-cast structure | tensile yield stress (MPa) | hardness (Hv) | $S_{\text{pred.}}$ (MPa) |
|------------------------|------------------|---------------------------|---------------|--------------------------|
| Nb [41]                | BCC              | 188                       | -             | 224.2                    |
| NbTi [41]              | BCC              | 354                       | -             | 367                      |
| NbTiZr [41 & 43]       | BCC              | 749 [41]-956 [43]         | 295 [43]      | 864.2                    |
| NbTiHf [41]            | BCC              | 613                       | -             | 492.2                    |
| NbTiZrHf [41]          | BCC              | 783                       | -             | 992.9                    |
| NbTaTiZr [41]          | BCC              | 876                       | -             | 962.8                    |
| NbTaTiHf [41]          | BCC              | 762                       | -             | 643.4                    |
| NbTaZrHf [41]          | BCC              | 1046                      | -             | 1186                     |
| NbTaTiZrHf [1]         | BCC              | 1142                      | -             | 1052                     |
| NbTa [42]              | BCC              | 246                       | -             | 575.9                    |
| HfNbTa [42]            | BCC              | 847                       | -             | 716.2                    |
| TiNbTa [42-43]         | BCC              | 478 [42]-620 [43]         | 246 [43]      | 505.2                    |
| TiHfNbTa [42]          | BCC              | 663                       | -             | 643.4                    |
| HfNbTaTiZr [43]        | BCC              | 1155                      | 359           | 1052                     |
| NbTaTiZr [43]          | BCC              | 1144                      | 358           | 962.8                    |
| Nb1.5TaTiZr0.5 [43]    | BCC              | 822                       | 294           | 804.2                    |
| AlNbTaTi [44]          | BCC              | -                         | 458$^1$       | 988.5                    |
| MoNbTaTi [44]          | BCC              | -                         | 431$^2$       | 1104                     |
| HfNbTaTi [44]          | BCC              | -                         | 270$^2$       | 643.4                    |
| AlMoNbTaTi [44]        | BCC              | -                         | 509$^2$       | 1479                     |
| Ti$_{38}$V$_{15}$Nb$_{23}$Hf$_{24}$ [45] | BCC      | 800                       | -             | 709.2                    |
| NbTiVZr$_{0.5}$ [46]   | BCC              | -                         | 340$^2$       | 1018                     |
| NbTiVZr [46]           | BCC              | -                         | 355$^2$       | 1125                     |
| NbTiVZr$_2$ [46]       | BCC              | -                         | 350$^2$       | 1085                     |
| Ti$_{45}$Zr$_{25}$Nb$_{25}$Ta$_{5}$ [47] | BCC | 790                       | -             | 872.6                    |
| Ti$_{40}$Zr$_{25}$Nb$_{25}$Ta$_{10}$ [47] | BCC | 910                       | -             | 896.4                    |
| Ti$_{35}$Zr$_{25}$Nb$_{25}$Ta$_{15}$ [47] | BCC | 1075                      | -             | 919.4                    |
| Ti$_{30}$Zr$_{25}$Nb$_{25}$Ta$_{20}$ [47] | BCC | 1150                      | -             | 941.5                    |
| TaZrHfTi [48]          | BCC              | 1356                      | -             | 1062                     |
| HfNbTiZr [49]          | BCC              | 636                       | -             | 992.9                    |
| TiVTa [50]             | BCC              | 801                       | -             | 782.1                    |
| Ti$_{40}$V$_{33}$Ta$_{27}$ [50] | BCC | 926                       | -             | 770.8                    |
| Ti$_{45}$V$_{20}$Ta$_{35}$ [50] | BCC | 838                       | -             | 702.5                    |
| Ti$_{48}$Zr$_{20}$Hf$_{15}$Al$_{10}$Nb$_7$ [51] | BCC | 675                       | -             | 1051                     |
| Ti$_{47}$Zr$_{20}$Hf$_{15}$Al$_{10}$Nb$_8$ [51] | BCC | 745                       | -             | 1052                     |
| Ti$_{46}$Zr$_{20}$Hf$_{15}$Al$_{10}$Nb$_9$ [51] | BCC | 700                       | -             | 1053                     |
| Zr$_{50}$Ti$_{35}$Nb$_{15}$ [52] | BCC | 657                       | -             | 699.7                    |
According to the results in Table 3, it can be seen that a relatively good agreement exists for quaternary and quinary alloy systems, but strength predictions for binary and ternary alloy systems are not accurate. That is probably because few experimental data related to these alloy systems are used for developing the polynomial. Furthermore, the V and Hf content of ternary alloys (33 at.%) is out of the composition domain in Figure 1. So, the predictions are not accurate for these alloys. If more experimental data for binary and ternary alloy systems can be provided, then a more accurate polynomial and, as a result, more accurate predictions can be obtained. According to the obtained results, it can be concluded that the developed polynomial can predict the strength of bcc RHEAs (not binary and ternary alloy systems) with a reasonable accuracy and therefore it can be considered as an easy-to-use tool for designing RHEAs. It should be noted although the approach used here is basically a curve fitting exercise and it does not consider the mechanisms involved in the strengthening of alloys, it can be considered as a straightforward method for assessing the strength of solid solution RHEAs in Al-Hf-Nb-Mo-Ta-Ti-V-Zr system.
4. Alloy design

To show how the developed polynomial can be applied in designing RHEAs, the alloy system Hf-Mo-Nb-Ta-Ti-V-Zr is selected as an example, and the strength of RHEAs within this system is predicted by developed polynomial. In this regard, an iterative MATLAB code is written and more than 40000 alloys with chemical compositions in the following range are examined $5 < \text{Hf} < 20$, $5 < \text{Mo} < 20$, $5 < \text{Nb} < 20$, $5 < \text{Ta} < 20$, $5 < \text{Ti} < 20$, $5 < \text{V} < 20$, and $5 < \text{Zr} < 20$. The relations between the concentrations of constituent elements and the strength of designed alloys in Hf-Mo-Nb-Ta-Ti-V-Zr system are shown in Figure 5. It can be observed that the strength increases with increasing the Mo and Zr contents and decreases with increasing the Ti content.
Figure 5. The effects of constituent elements on the strength of designed RHEAs in Hf-Mo-Nb-Ta-Ti-V-Zr system (the trends are shown with red lines)
In general, two approaches can be considered for explaining the effect of alloying elements in HEAs [5]. The first approach is according to the Labusch theory [5, 53] which model the solid solution strengthening mechanism by considering the interactions between the dislocations and the non-homogeneities of a lattice. This approach is used in [8, 12, 20, 29, 54-56]. In the second approach, the non-homogeneities of the lattice are considered within the core of dislocations and the solid solution strengthening mechanism is explained by enhanced Peierls-Nabarro stress ($\sigma_{PN}$) or friction stress ($\sigma_f$) of the lattice. This approach is used in [41, 57-60].

The effect of Mo and Zr on the strength of alloys may be explained by considering the Labusch theory [5, 53]. According to the Labusch theory, the strengthening degree of an element depends on the atomic size and elastic modulus mismatches between the solute and solvent, and the strengthening increases with increasing the amount of mismatches. Mo has a relatively low atomic radius in comparison with other constituent elements in Hf-Mo-Nb-Ta-Ti-V-Zr system ($r_{Mo}= 1.362$ Å, $r_{avg}= 1.454$ Å) (Table 4). Furthermore, Mo has the highest Young's modulus among the constituent elements. Therefore, when Mo is introduced to the lattice, high atomic size and elastic modulus mismatches are expected which will cause a high degree of strengthening effect for Mo. This may be the reason for the strengthening effect observed for Mo in Figure 5. On the other hand, Zr has the highest atomic radius among the constituent elements which can cause high atomic size mismatches leading to the strengthening effect for Zr as it can be seen in Figure 5.
Table 4. Elements properties

| Element | Crystal structure (RT) [3] | Young's Modulus (GPa) [3] | Shear Modulus (GPa) [20] | Yield stress (Polycrystal) (MPa) | VEC [3] | Atom radius (pm) [3] |
|---------|----------------------------|---------------------------|--------------------------|---------------------------------|--------|---------------------|
| Hf      | hcp                        | 78                        | 30                       | 200 [48]                        | 4      | 157.75              |
| Mo      | bcc                        | 329                       | 120                      | 438 [27]                        | 6      | 136.26              |
| Nb      | bcc                        | 105                       | 38                       | 240 [27]                        | 5      | 142.9               |
| Ta      | bcc                        | 186                       | 69                       | 345 [27]                        | 5      | 143                 |
| Ti      | hcp                        | 116                       | 44                       | 195 [27]                        | 4      | 146.15              |
| V       | bcc                        | 128                       | -                        | 310 [27]                        | 5      | 131.6               |
| Zr      | hcp                        | 68                        | 33                       | 160 [48]                        | 4      | 160.25              |

The softening behavior of Ti cannot be explained by considering the atomic radius or elastic modules of Ti. One speculation for the softening effect observed for Ti could be its effect in lowering the Peierls-Nabarro stress (PN stress) as a result of reducing the directionality of the electron bondings due to the lower valence electron concentration (VEC) of Ti [39, 61-63]. As it can be seen in Table 4, hcp metals with valence electron concentration (VEC) of 4 have in general lower yield stresses in comparison with bcc metals with VEC of 5. Furthermore, it can be seen that Mo with VEC of 6 has the highest yield stress in comparison to other elements. So, it may be concluded that a relationship exists between VEC and the strength of alloys. This hypothesis is examined for designed RHEAs, and Figure 6 shows the relation between VEC and compressive yield stress of designed alloys. It can be seen that a trend exists between VEC and the compressive yield stress of alloys and strength increases with increasing VEC. Therefore, the softening behavior of Ti might be due to its low VEC and its effect on lowering the PN stress. Softening behavior of Ti is reported for Al-Cr-Nb-Ti alloys as well [64-66]. It is reported that Ti increases the fracture toughness of Al-Cr-Nb-Ti alloys by
increasing dislocation mobility through a reduction of the PN energy and stress [64-66].

![Graph showing the relation between valence electron concentration (VEC) and predicted compressive yield stress of designed alloys.](image)

**Figure 6.** The relation between valence electron concentration (VEC) and predicted compressive yield stress of designed alloys

The solid solution strengthening effect in HEAs can also be assessed by the parameter atomic size difference (ASD) [5] which can be evaluated by the following equation [5]

$$ASD = \sqrt{\sum_{i=1}^{N} C_i \left(1 - \frac{r_i}{\bar{r}}\right)^2}$$

where $C_i$ and $r_i$ are the atomic fraction and atomic radius of element $i$ respectively and $\bar{r}$ is the composition-weighted average atomic radius ($\bar{r} = \sum_{i=1}^{N} C_i r_i$). The relation between ASD and the compressive yield stress of designed alloys is shown in Figure 7. As it can be seen a correlation exists between ASD and the compressive yield stress of alloys, and the strength
increases with increasing ASD. Therefore, ASD should be maximized for designing stronger solid solution alloys.

Figure 7. The relation between atomic size difference (ASD) and predicted compressive yield stress of designed alloys

According to the results in Figures 6 and 7, it can be seen that parameters VEC and ASD can affect the strength of RHEAs. Other parameters which can affect the strength of a solid solution alloy are elastic modules [5], lattice distortion [41], electronegativity differences [67] and short range orders [68]. In order to investigate the effect of an alloying element, these parameters should be considered simultaneously. Therefore, the role of a constituent element in changing the strength (Figure 5) may be explained by considering the role of that element in changing the above parameters and how changing the above parameters can affect the strength (strengthening or softening). It should be mentioned that the results in Figure 5 are only valid for the alloy system Hf-Mo-Nb-Ta-Ti-V-Zr and within the investigated composition range. With changing the
alloy system or the concentration of constituent elements the effect of constituent elements on strength may change.

The hardest alloy in Hf-Mo-Nb-Ta-Ti-V-Zr system within the investigated composition range is predicted to be Hf$_{15}$Mo$_{20}$Nb$_{5}$Ta$_{15}$Ti$_{5}$V$_{20}$Zr$_{20}$ with the yield stress of 1792 MPa. According to the tensile-ductility data in previous research works [34, 41-52], alloys with tensile yield stresses less than 1200 MPa could have tensile ductility higher than 5% (Figure 8). Therefore, the developed polynomial is used for finding alloys in Hf-Mo-Nb-Ta-Ti-V-Zr system with compressive yield stresses less than 1150 MPa. Around 80 alloys where found and the list of these alloys can be seen in Appendix A (Table A1). Some tensile ductility may be expected for alloys in Table A1. On the other hand, all of the alloys in Table A1 have melting temperatures higher 2400 °C (rule of mixture is used for predicting the melting temperatures). Furthermore, according to the recently published paper by Senkov et. al. [69], the loss of high-temperature strength of single-phase bcc RHEs occurs at temperatures higher than 0.6 T$_m$ [69]. Therefore, it may be predicted that alloys in Table A1 keep their strength up to temperatures around 1300 °C (0.6 T$_m$) which is high enough for most of the application. Therefore, reasonable room temperature (ductility) and high temperature mechanical properties may be expected for alloys in Table A1.
Figure 8. Tensile ductility versus tensile yield stress for single-phase bcc RHEs [34, 41-52]

Similar to the procedure used for investigating the RHEAs in Hf-Mo-Nb-Ta-Ti-V-Zr system, other alloys systems may also be investigated and the strongest alloy in each alloy system can be identified. Although the predictions may not be very accurate, but they can be considered as good estimates of strength values. Considering the large composition domain which exists within the central regions of multicomponent phase diagrams, and the vast number of alloys which can be selected, even having estimates of strength values can be very valuable. Therefore, the developed polynomial can be considered as a valuable tool in designing of RHEAs. The developed approach can also be used for other alloy systems. For example, the author applied the same approach for predicting the hardness of face centered cubic (fcc) solid solution HEAs in Co-Cr-Fe-Mn-Ni system [70] and it is observed that the polynomial equation could model the hardness of solid solution Co-Cr-Fe-Mn-Ni alloys very well [71].
At the end few points need to be mentioned about the developed polynomial. 1- The microstructures (including parameters such as grain size, porosity and micro segregations) of alloys in Table 1 were not the same although all of them were made by vacuum arc melting technique. Furthermore, the mechanical testing conditions were not exactly the same. So, it may not be accurate to compare the yield stress values in Table 1 just based on the chemical compositions, and microstructural parameters should also be considered; Therefore, it is more reasonable to assume some degree of deviation for the yield stress values in Table 1. If these deviations can be considered, then a more accurate polynomial can be obtained. Nevertheless, it was observed that the developed polynomial was able to estimate the yield stress values with a reasonable accuracy by just using the alloy composition as input. If experimental data can be provided for alloys with the same preparation and microstructural conditions, then more accurate results can be obtained. 2- If more experimental data can be provided, then a more accurate polynomial can be developed; furthermore, if more experimental data can be provided then the composition domain (Figure 1) within which the polynomial is valid can be expanded. According to the relatively fast growing field of RHEAs, more experimental data are expected to be available which could be used for improving the accuracy of the polynomial. Moreover, if reasonable number of data can be provided for alloys containing Cr and W, then the polynomial can be further improved to cover RHEAs alloys containing Cr and W. 3- Other forms of equations may be used for modeling the strength of solid solution alloys, and more accurate results may be obtained. For example, one may develop equations based on parameters $C^{1/2}$ and $C^{3/2}$ according to Labusch theory instead of using parameters $C$ and $C^2$. 
5. Conclusions

In summary, a simple polynomial equation is used to model the compressive yield stress of as-cast solid solution refractory high entropy alloys in Al-Hf-Mo-Nb-Ta-Ti-V-Zr system. More than 80 experimental data are used for finding the polynomial’s coefficients. The results show that the proposed polynomial could model the yield strength of solid solution alloys with a reasonable accuracy. The developed polynomial is used for predicting the strength of RHEAs in Hf-Mo-Nb-Ta-Ti-V-Zr system. The results show that the strength of designed alloys increases with increasing the value of parameters valence electron concentration (VEC) and atomic size difference (ASD). Furthermore, the results show that for investigated alloy system, Mo and Zr have both strengthening effect while Ti shows softening effect.
6. References

[1] E. P. George, D. Raabe, R. O. Ritchie, High-entropy alloys, Nature Reviews Materials, 2019, 4, 515-534

[2] D. B. Miracle, High entropy alloys as a bold step forward in alloy development, Nature Communications, 2019, 10, article number: 1805

[3] D. B. Miracle, O. N. Senkov, A critical review of high entropy alloys and related concepts, Acta Materialia, 2017, 122, 448-511

[4] Y.F. Ye, Q. Wang, J. Lu, C.T. Liu, Y. Yang, High-entropy alloy: challenges and prospects, Materials Today, 2016, 19(6), 349-362

[5] O. N. Senkov, D. B. Miracle, K. J. Chaput, J. P. Couzinie, Development and exploration of refractory high entropy alloys – review, Journal of Materials Research, 2018, 33, 3092-3128

[6] O.N. Senkov, G.B. Wilks, D.B. Miracle, C.P. Chuang, P.K. Liaw, Refractory high-entropy alloys, Intermetallics, 2010, 18, 1758

[7] C. M. Lin, C. C. Juan, C. H. Chang, C. W. Tsai, J. W. Yeh, Effect of Al addition on mechanical properties and microstructure of refractory AlxHfNbTaTiZr alloys, Journal of Alloys and Compounds, 2015, 624, 100-107

[8] C. C. Juan, K. K. Tseng, W. L. Hsu, M. H. Tsai, C. W. Tsai, C. M. Lin, S. K. Chen, S. J. Lin, J. W. Yeh, Solution strengthening of ductile refractory HfMoxNbTaTiZr high-entropy alloys, Materials Letters, 2016, 175, 284-287

[9] Y. D. Wu, Y. H. Cai, T. Wang, J. J. Si, J. Zhu, Y. D. Wang, X. D. Hui, A refractory Hf25Nb25Ti25Zr25 high-entropy alloy with excellent structural stability and tensile properties, Materials Letters, 2014, 130, 277-280

[10] G. Dirras, L. Lilenstein, P. Djemia, M. Laurent-Brocq, D. Tingaud, J. P. Couzinié, L. Perrière, T. Chauveau, I. Guillot, Elastic and plastic properties of as-cast equimolar TiHfZrTaNb high-entropy alloy, Materials Science and Engineering: A, 2016, 654, 30-38

[11] S. Sheikh, S. Shafeie,Q. Hu, J. Ahlstrom, C. Persson, J. Vesely, J. Zyka, U. Klement, S. Guo, Alloy design for intrinsically ductile refractory high-entropy alloys, Journal of applied physics, 2016, 120, 164902
[12] F. G. Coury, M. Kaufman, A. J. Clarke, Solid-solution strengthening in refractory high entropy alloys, Acta Materialia, 2019, 175, 66-81

[13] C. C. Juan, M. H. Tsai, C. W. Tsai, C. M. Lin, W. R. Wang, C. C. Yang, S. K. Chen, S. J. Lin, J. W. Yeh, Enhanced mechanical properties of HfMoTaTiZr and HfMoNbTaTiZr refractory high-entropy alloys, Intermetallics, 2015, 62, 76-83

[14] O.N. Senkov, S.I. Rao, T.M. Butler, K.J. Chaput, Ductile Nb alloys with reduced density and cost, Journal of Alloys and Compounds, 2019, 808, 151685

[15] M. Feuerbacher, M. Heidelmann, C. Thomas, Plastic deformation properties of Zr–Nb–Ti–Ta–Hf high-entropy alloys, Philosophical Magazine, 2015, 95 (11), 1221-1232

[16] N.N. Guo, L. Wang, L.S. Luo, X.Z. Li, R.R. Chen, Y.Q. Su, J.J. Guo, H.Z. Fu, Microstructure and mechanical properties of refractory high entropy (Mo0.5Nb0.5Zr0.5Ti)BCC/M5Si3 in-situ compound, Journal of alloys and compounds, 2016, 660, 197-203

[17] N.N.Guo, L.Wang, L.S.Luo, X.Z.Li, Y.Q.Su, J.J.Guo, H.Z.Fu, Microstructure and mechanical properties of refractory MoNbHfZrTi high-entropy alloy, Materials & Design, 2015, 81, 87-94

[18] S. Maiti, W. Steurer, Structural-disorder and its effect on mechanical properties in single-phase TaNbHfZr high-entropy alloy, Acta Materialia, 2016, 106, 87-97

[19] Y. Zhang, X. Yang, P. K. Liaw, Alloy design and properties optimization of high-entropy alloys, JOM, 2012, 64(7), 830-838

[20] K. K. Tseng, C. C. Juan, S. Tso, H. C. Chen, C. W. Tsai, J. W. Yeh, Effects of Mo, Nb, Ta, Ti, and Zr on mechanical properties of equiatomic Hf-Mo-Nb-Ta-Ti-Zr alloys, Entropy, 2019, 21(1), 15

[21] Y. Chen, Y. Li, X. Cheng, C. Wu, B. Cheng, Z. Xu, The microstructure and mechanical properties of refractory high-entropy alloys with high plasticity, Materials, 2018, 11(2), 208

[22] T. Hori, T. Nagase, M. Todai, A. Matsugaki, T. Nakano, Development of non-equiaxial Ti-Nb-Ta-Zr-Mo high-entropy alloys for metallic biomaterials, Scripta Materialia, 2019, 172, 83-87
[23] Z. Q. Xu, Z. L. Ma, M. Wang, Y. W. Chen, Y. D. Tan, X. W. Cheng, Design of novel low-density refractory high entropy alloys for high temperature applications, Materials Science & Engineering A, 2019, 755, 318-322

[24] S. Y. Chen, X. Yang, K. A. Dahmen, P. K. Liaw, Y. Zhang, Microstructures and crackling noise of AlxNbTiMoV high entropy alloys, Entropy 2014, 16, 870-884

[25] D. Qiao, H. Jiang, X. Chang, Y. Lub, T. Li, Microstructure and mechanical properties of VTaTiMoAlx refractory high entropy alloys, Materials science forum, 2017, 898, 638-642

[26] Y. D. Wu, Y. H. Cai, X. H. Chen, T. Wang, J. J. Si, L. Wang, Y. D. Wang, X. D. Hui, Phase composition and solid solution strengthening effect in TiZrNbMoV high-entropy alloys, Materials and Design, 2015, 83, 651-660

[27] H. W. Yao, J. W. Qiao, J. A. Hawk, H. F. Zhou, M. W. Chen, M. C. Gao, Mechanical properties of refractory high-entropy alloys: experiments and modeling, Journal of Alloys and Compounds, 2017, 696, 1139-1150

[28] H. Yao, J. W. Qiao, M. C. Gao, J. A. Hawk, S. G. Ma, H. Zhou, MoNbTaV medium-entropy alloy, Entropy, 2016, 18, 189

[29] H. W. Yao, J. W. Qiao, M. C. Gao, J. A. Hawk, S. G. Mad, H. F. Zhou, Y. Zhang, NbTaV-(Ti,W) refractory high-entropy alloys : Experiments and modeling, Materials Science & Engineering A, 2016, 674, 203-211

[30] D. X. Qiao, H. Jiang, W. N. Jiao, Y. P. Lu, Z. Q. Cao, T. J. Li, A Novel series of refractory high-entropy alloys Ti2ZrHf0.5VNbx with high specific yield strength and good ductility, Acta Metallurgica Sinica (English Letters), 2019, 32, 925-931

[31] V.T. Nguyen, M. Qian, Z. Shi, T. Song, L. Huang, J. Zou, A novel quaternary equiatomic Ti-Zr-Nb-Ta medium entropy alloy (MEA), Intermetallics, 2018, 101, 39-43

[32] Y. M. Hu, X. D. Liu, N. N. Guo, L. Wang, Y. Q. Su, J. J. Guo, Microstructure and mechanical properties of NbZrTi and NbHfZrTi alloys, Rare Metals, 2019, 38 (9), 840-847

[33] Q. Li, H. Zhang, D. Li, Z. Chen, F. Wang, M. Wu, Comparative study of the microstructures and mechanical properties of laser metal deposited and vacuum arc melted refractory NbMoTa medium-entropy alloy, International Journal of Refractory Metals and Hard Materials, 2020, https://doi.org/10.1016/j.ijrmhm.2020.105195

25
[34] Y. Yuan, Y. Wu, Z. Yang, X. Liang, Z. Lei, H. Huang, H. Wang, X. Liu, K. An, W. Wu, Z. Lu, Formation, structure and properties of biocompatible TiZrHfNbTa high-entropy alloys, Materials Research Letters, 2019, 7 (6), 225-231

[35] S. Ozan, J. Lin, Y. Li, R. Ipek, C. Wena, Development of Ti–Nb–Zr alloys with high elastic admissible strain for temporary orthopedic devices, Acta Biomaterialia, 2015, 20, 176-187

[36] L. B. Zhang, K. Z. Wang, L. J. Xu, S. L. Xiao, Y. Y. Chen, Effect of Nb addition on microstructure, mechanical properties and castability of β-type Ti-Mo alloys, Trans. Nonferrous Met. Soc. China, 2015, 25, 2214-2220

[37] P. Li, X. Ma, T. Tong, Y. Wang, Microstructural and mechanical properties of β-type TiMoNb biomedical alloys with low elastic modulus, Journal of Alloys and Compounds, 2020, 815, 152412

[38] B. C. Peters, A. Hendrickson, The strength of tantalum columbium alloy single crystals, Acta Metallurgica, 1966, 14 (9), 1121-1122

[39] J. R. Stephens, W. R. Witzke, Alloy hardening and softening in binary molybdenum alloys as related to electron concentration, Journal of the less common metals, 1972, 29, 371-388

[40] D. L. Harrod and R. E. Gold, Mechanical properties of vanadium and vanadium-base alloys, International Metals Reviews, 1980, 25 (1), 163-222

[41] Y. Y. Zhao, Z. F. Lei, Z. P. Lu, J. C. Huang, T. G. Nieh, A simplified model connecting lattice distortion with friction stress of Nb-based equiatomic high entropy alloys, Materials Research Letters, 2019, 7(8), 340-346

[42] S. P. Wang, E. Mac, J. Xu, New ternary equi-atomic refractory medium-entropy alloys with tensile ductility: Hafnium versus titanium into NbTa-based solution, Intermetallics, 2019, 107, 15-23,

[43] J. Zyka, J. Malek, J. Vesely, F. Lukac, J. Cizek, J. Kuriplach, O. Melikhova, Microstructure and room temperature mechanical properties of different 3 and 4 element medium entropy alloys from HfNbTaTiZr system, Entropy, 2019, 21, 114

[44] F. G. Coury, T. Butler, K. Chaput, A. Saville, J. Copley, J. Foltz, P. Mason, K. Clarke, M. Kaufman, A. Clarke, Phase equilibria, mechanical properties and design of quaternary refractory high entropy alloys, Materials & Design, 2018, 155, 244-256
[45] arXiv:1911.10975

[46] D. J. M. King, S. T. Y. Cheung, S. A. Humphry-Baker, C. Parkin, A. Couet, M. B. Cortie, G.R. Lumpkin, S. C. Middleburgh, A. J. Knowles, High temperature, low neutron cross-section high-entropy alloys in the Nb-Ti-V-Zr system, Acta Materialia, 2019, 166, 435-446

[47] V. T. Nguyen, M. Qian, Z. Shi, T. Song, L. Huang, J. Zou, Compositional design of strong and ductile (tensile) Ti-Zr-Nb-Ta medium entropy alloys (MEAs) using the atomic mismatch approach, Materials Science and Engineering: A, 2019, 742, 762-772

[48] H. Huang, Y. Wu, J. He, H. Wang, X. Liu, K. An, W. Wu, Z. Lu, Phase-transformation ductilization of brittle high-entropy alloys via metastability engineering, Advanced Materials, 2017, 29 (30), 1701678

[49] Y. Ma, S. Wu, Y. Jia, P. Hu, Y. Bu, X. Chen, G. Wang, J. Liu, H. Wang, Q. Zhai, Hexagonal closed-packed precipitation enhancement in a NbTiHfZr refractory high-entropy alloy, Metals, 2019, 9, 485

[50] N. Jia, Y. Lli, X. Liu, Y. Zheng, B. Wang, J. Wang, Y. Xue, K. Jin, Thermal stability and mechanical properties of low-activation single-phase Ti-V-Ta medium entropy alloys, JOM, 2019, 71 (10), 3490-3498

[51] L. Wang, C. Fu, Y. Wu, Q. Wang, X. Hui, Y. Wang, Formation and toughening of metastable phases in TiZrHfAlNb medium entropy alloys, Materials Science and Engineering: A, 2019, 748, 441-452

[52] X. Yan, Y. Zhang, A body-centered cubic Zr50Ti35Nb15 medium-entropy alloy with unique properties, Scripta Materialia, 2020, 178, 3293-333

[53] R. Labusch, A statistical theory of solid solution hardening, Physica Status Solidi (b), 1970, 41 (2), 659-669

[54] O.N. Senkov, J.M. Scott, S.V. Senkova, D.B. Miracle, C.F. Woodward, Microstructure and room temperature properties of a high-entropy TaNbHfZrTi alloy, Journal of Alloys and Compounds, 2011, 509, 6043-6048

[55] I. Toda-Caraballo and P. E. J. Rivera-Diaz-del-Castillo, Modelling solid solution hardening in high entropy alloys, Acta Materlia, 2015, 85, 14-23

[56] I. Toda-Caraballo and P. E. J. Rivera-Diaz-del-Castillo, Modelling solid solution hardening in high entropy alloys, Acta Materlia, 2015, 85, 14-23

27
[57] L. Zhang, Y. Xiang, J. Han, D. J. Srolovitz, The effect of randomness on the strength of high-entropy alloys, Acta Materialia, 2019, 166, 424-434

[58] X. Liu, Z. Pei, M. Eisenbach, Dislocation core structures and Peierls stresses of the high-entropy alloy NiCoFeCrMn and its subsystems, Materials and Design, 2019, 180, 107955

[59] Y.Y. Zhao, T.G. Nieh, Correlation between lattice distortion and friction stress in Ni-based equiatomic alloys, Intermetallics, 2017, 86, 45-50

[60] S. S. Sohn, A. K. Silva, Y. Ikeda, F. Körmann, W. Lu, W. S. Choi, B. Gault, D. Ponge, J. Neugebauer, D. Raabe, Ultrastrong medium-entropy single-phase alloys designed via severe lattice distortion, Advanced Materials, 2019, 31 (8), 1807142

[61] J. R. Stephens, W. R. Witzke, The role of electron concentration in softening and hardening of ternary molybdenum alloys, Journal of the Less Common Metals, 1975, 41 (2), 265-282

[62] Y. Hiraoka, T. Ogusu, N. Yoshizawa, Decrease of yield strength in molybdenum by adding small amounts of Group VIII elements, Journal of Alloys and Compounds, 2004, 381(1-2), 192-196

[63] G. D. Samolyuk, Y. N. Osetsky, R. E. Stoller, The influence of transition metal solutes on the dislocation core structure and values of the Peierls stress and barrier in tungsten, Journal of Physics: Condensed Matter, 2013, 25, 025403

[64] K. S. Chan, D. L. Davidson, Effects of Ti addition on cleavage fracture in Nb-Cr-Ti solid-solution alloys, Metallurgical and Materials Transactions A, 1999, 30(4), 925-939

[65] K. S. Chan, A computational approach to designing ductile Nb-Ti-Cr-Al solid-solution alloys, Metallurgical and Materials Transactions A, 2001, 32(10), 2475-2487

[66] D. L. Davidson, K. S. Chan, D. L. Anton, The effects on fracture toughness of ductile-phase composition and morphology in Nb-Cr-Ti and Nb-Si in situ composites, Metallurgical and Materials Transactions A, 1996, 27 (10), 3007-3018

[67] H. S. Oh, S. J. Kim, K. Odbadrakh, W. H. Ryu, K. N. Yoon, S. Mu, F. Körmann, Y. Ikeda, C. C. Tasan, D. Raabe, T. Egami, E. S. Park, Engineering atomic-level complexity in high-entropy and complex concentrated alloys, Nature Communications, 2019, 10, 2090
[68] Q. J. Li, H. Sheng, E. Ma, Strengthening in multi-principal element alloys with local-chemical-order roughened dislocation pathways, Nature Communications, 2019, 10, 3563

[69] O.N. Senkov, S. Gorsse, D.B. Miracle, High temperature strength of refractory complex concentrated alloys, Acta Materialia, 2019, 175, 394-405

[70] G. Bracq, M. Laurent-Brocq, C. Varvenne, L. Perrière, W.A. Curtin, J. M. Joubert, I. Guillot, Combining experiments and modelling to explore the solid solution strengthening of high and medium entropy alloys, Acta Materialia, 2019, 177, 1, 266-279

[71] A. Shafieie, A new approach to model the strength of solid-solution high entropy alloys in Co-Cr-Fe-Mn-Ni system, submitted
Appendix A

Table A1. Designed alloys with melting point higher than 2400°C and yield stress less than 1150 MPa (melting points are calculated by the rule of mixture and yield stress values are predicted by developed polynomial)

| Hf | Mo | Nb  | Ta  | Ti  | V  | Zr | $T_m$ (°C) | S(MPa) |
|----|----|-----|-----|-----|----|----|-----------|--------|
| 10 | 5  | 20  | 20  | 20  | 20 | 5  | 2534.6    | 1120.955 |
| 12.5 | 5 | 17.5 | 20  | 20  | 20 | 5  | 2528.5    | 1134.21  |
| 12.5 | 5 | 20  | 17.5 | 20  | 20 | 5  | 2515      | 1128.221 |
| 12.5 | 5 | 20  | 20  | 17.5 | 20 | 5  | 2548.725  | 1143.108 |
| 12.5 | 5 | 20  | 20  | 20  | 17.5 | 5 | 2542.675  | 1114.629 |
| 15  | 5  | 15  | 20  | 20  | 20 | 5  | 2522.4    | 1143.265 |
| 15  | 5  | 17.5 | 17.5 | 20  | 20 | 5  | 2508.9    | 1137.901 |
| 15  | 5  | 17.5 | 17.5 | 20  | 17.5 | 5 | 2536.575  | 1124.309 |
| 15  | 5  | 20  | 15  | 20  | 20 | 5  | 2495.4    | 1130.925 |
| 15  | 5  | 20  | 20  | 17.5 | 20  | 5 | 2529.125  | 1146.799 |
| 15  | 5  | 20  | 20  | 20  | 17.5 | 5 | 2523.075  | 1118.32  |
| 15  | 5  | 20  | 20  | 17.5 | 17.5 | 5 | 2556.8    | 1133.206 |
| 15  | 5  | 20  | 20  | 20  | 12.5 | 7.5 | 2549.375  | 1137.256 |
| 15  | 5  | 20  | 20  | 20  | 15  | 5  | 2550.75   | 1102.69  |
| 15  | 7.5 | 20  | 20  | 20  | 12.5 | 5 | 2568.575  | 1146.651 |
| 17.5 | 5 | 12.5 | 20  | 20  | 20 | 5  | 2516.3    | 1148.12  |
| 17.5 | 5 | 15  | 17.5 | 20  | 20 | 5  | 2502.8    | 1143.381 |
| 17.5 | 5 | 15  | 20  | 20  | 17.5 | 5 | 2530.475  | 1129.789 |
| 17.5 | 5 | 17.5 | 15  | 20  | 20 | 5  | 2489.3    | 1137.03  |
| 17.5 | 5 | 17.5 | 17.5 | 20  | 17.5 | 5 | 2516.975  | 1124.425 |
| 17.5 | 5 | 17.5 | 20  | 17.5 | 17.5 | 5 | 2550.7    | 1139.311 |
| 17.5 | 5 | 17.5 | 20  | 20  | 12.5 | 7.5 | 2543.275  | 1143.361 |
| 17.5 | 5 | 17.5 | 20  | 20  | 15  | 5  | 2544.65   | 1108.795 |
| 17.5 | 5 | 20  | 12.5 | 20  | 20 | 5  | 2475.8    | 1129.066 |
| 17.5 | 5 | 20  | 15  | 17.5 | 20  | 5 | 2509.525  | 1145.928 |
| 17.5 | 5 | 20  | 15  | 20  | 17.5 | 5 | 2503.475  | 1117.449 |
| 17.5 | 5 | 20  | 17.5 | 17.5 | 17.5 | 5 | 2537.2    | 1133.323 |
| 17.5 | 5 | 20  | 17.5 | 20  | 12.5 | 7.5 | 2529.775  | 1137.373 |
| 17.5 | 5 | 20  | 17.5 | 20  | 15  | 5 | 2531.15   | 1102.806 |
| 17.5 | 5 | 20  | 20  | 17.5 | 17.5 | 5 | 2570.925  | 1148.984 |
| 17.5 | 5 | 20  | 20  | 17.5 | 15  | 5 | 2564.875  | 1117.693 |
| 17.5 | 5 | 20  | 20  | 20  | 7.5 | 10 | 2556.075  | 1142.234 |
| 17.5 | 5  | 20 | 20 | 20 | 10 | 7.5 | 2557.45 | 1117.668 |
|------|----|----|----|----|----|-----|--------|---------|
| 17.5 | 5  | 20 | 20 | 20 | 12.5| 5   | 2558.825| 1085.139|
| 17.5 | 7.5| 20 | 17.5| 20 | 12.5| 5   | 2548.975| 1146.768|
| 17.5 | 7.5| 20 | 20 | 20 | 10  | 5   | 2576.65 | 1127.063|
| 20   | 5  | 10 | 20 | 20 | 20  | 5   | 2510.2  | 1148.775|
| 20   | 5  | 12.5| 17.5| 20 | 20  | 5   | 2496.7  | 1144.661|
| 20   | 5  | 12.5| 20 | 20 | 17.5| 5   | 2524.375| 1131.069|
| 20   | 5  | 15  | 15 | 20 | 20  | 5   | 2483.2  | 1138.935|
| 20   | 5  | 15  | 17.5| 20 | 17.5| 5   | 2510.875| 1126.33 |
| 20   | 5  | 15  | 17.5| 20 | 17.5| 7.5 | 2544.6  | 1141.216|
| 20   | 5  | 15  | 20 | 20 | 12.5| 7.5 | 2537.175| 1145.266|
| 20   | 5  | 15  | 20 | 20 | 15  | 5   | 2538.55 | 1110.7  |
| 20   | 5  | 17.5| 12.5| 20 | 20  | 5   | 2469.7  | 1131.596|
| 20   | 5  | 17.5| 15  | 17.5| 20  | 5   | 2503.425| 1148.458|
| 20   | 5  | 17.5| 15  | 20 | 17.5| 5   | 2497.375| 1119.979|
| 20   | 5  | 17.5| 17.5| 20 | 17.5| 5   | 2531.1  | 1135.853|
| 20   | 5  | 17.5| 17.5| 20 | 12.5| 7.5 | 2523.675| 1139.903|
| 20   | 5  | 17.5| 17.5| 20 | 15  | 5   | 2525.05 | 1105.336|
| 20   | 5  | 17.5| 17.5| 15 | 15  | 5   | 2558.775| 1120.223|
| 20   | 5  | 17.5| 20  | 17.5| 20  | 5   | 2549.975| 1144.764|
| 20   | 5  | 17.5| 20  | 20 | 10  | 7.5 | 2551.35 | 1120.198|
| 20   | 5  | 17.5| 20  | 20 | 12.5| 5   | 2552.725| 1087.669|
| 20   | 5  | 20  | 10  | 20 | 20  | 5   | 2456.2  | 1122.645|
| 20   | 5  | 20  | 12.5| 17.5| 20  | 5   | 2489.925| 1140.494|
| 20   | 5  | 20  | 12.5| 20 | 15  | 7.5 | 2482.5  | 1148.619|
| 20   | 5  | 20  | 12.5| 20 | 17.5| 5   | 2483.875| 1112.015|
| 20   | 5  | 20  | 15  | 17.5| 17.5| 5   | 2517.6  | 1128.876|
| 20   | 5  | 20  | 15  | 20 | 12.5| 7.5 | 2510.175| 1132.926|
| 20   | 5  | 20  | 15  | 20 | 15  | 5   | 2511.55 | 1098.36 |
| 20   | 5  | 20  | 17.5| 15 | 17.5| 5   | 2551.325| 1145.525|
| 20   | 5  | 20  | 17.5| 17.5| 12.5| 7.5 | 2543.9  | 1148.8  |
| 20   | 5  | 20  | 17.5| 17.5| 15  | 5   | 2545.275| 1114.234|
| 20   | 5  | 20  | 17.5| 20 | 7.5  | 10  | 2536.475| 1138.775|
| 20   | 5  | 20  | 17.5| 20 | 10  | 7.5 | 2537.85 | 1114.209|
| 20   | 5  | 20  | 17.5| 20 | 12.5| 5   | 2539.225| 1081.68 |
| 20   | 5  | 20  | 20 | 15  | 15  | 5   | 2579    | 1129.895|
| 20   | 5  | 20  | 20 | 17.5| 10  | 7.5 | 2571.575| 1129.095|
| 20   | 5  | 20  | 20 | 17.5| 12.5| 5   | 2572.95 | 1096.566|
| 20   | 5  | 20  | 20 | 20  | 5   | 10  | 2564.15 | 1114.995|
| 20   | 5  | 20  | 20 | 20 | 7.5  | 7.5 | 2565.525| 1092.466|
| 20   | 5  | 20  | 20 | 20 | 10  | 5   | 2566.9  | 1061.975|

31
| 20 | 7.5 | 17.5 | 17.5 | 20 | 12.5 | 5 | 2542.875 | 1149.298 |
|----|-----|------|------|----|------|---|-----------|----------|
| 20 | 7.5 | 17.5 | 20 | 20 | 10 | 5 | 2570.55 | 1129.593 |
| 20 | 7.5 | 20 | 15 | 20 | 12.5 | 5 | 2529.375 | 1142.321 |
| 20 | 7.5 | 20 | 17.5 | 20 | 10 | 5 | 2557.05 | 1123.604 |
| 20 | 7.5 | 20 | 20 | 17.5 | 10 | 5 | 2590.775 | 1138.49 |
| 20 | 7.5 | 20 | 20 | 20 | 5 | 7.5 | 2583.35 | 1130.315 |
| 20 | 7.5 | 20 | 20 | 20 | 7.5 | 5 | 2584.725 | 1101.861 |
| 20 | 10 | 20 | 20 | 20 | 5 | 5 | 2602.55 | 1135.66 |