SIMPLE APPROACH TO MODEL THE STRENGTH OF SOLID-SOLUTION HIGH ENTROPY ALLOYS IN Co-Cr-Fe-Mn-Ni SYSTEM

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A simple fitting approach is introduced for modeling the strength (hardness) of quaternary and quinary face-centered cubic (fcc) solid solution high entropy alloys (HEAs) in the Co-Cr-Fe-Mn-Ni system. The strength of solid solution HEAs could be modeled by a polynomial equation where experimental data are used to find the polynomial coefficients. It is observed that the proposed polynomial could model the strength of solid solution HEAs very well. Effects of constituent elements on the hardness of quinary Co-Cr-Fe-Mn-Ni alloys are investigated; the results indicate that alloys’ strength decreases with the Fe content. The softening effect of Fe is explained by considering its impact on reducing the shear modulus of alloys. Furthermore, the effects of parameters enthalpy of mixing and valence electron concentration on the strength of HEAs are investigated. The results show that the enthalpy of mixing has a noticeable impact on the hardness of quinary Co-Cr-Fe-Mn-Ni alloys, and the strength increases with decreasing the enthalpy of mixing. Furthermore, the results show that quinary Co-Cr-Fe-Mn-Ni alloys’ hardness increases with the parameter valence electron concentration.

Keywords: hardness, microstructure, metal and alloys, modeling, high entropy alloys.

Introduction. Multi-principal element or multi-component alloys with at least three principal elements (e. g., CoCrNi or CoCrFeMnNi) have received wide attention recently because they may have enhanced properties in comparison with traditional alloys, which are usually based on one dominant element [1, 2]. While these alloys contain several principal elements, sometimes they crystallize in single-phase solid solutions with simple crystal structures. The occurrence of alloys with single-phase solid solutions is attributed to high configurational entropies of random solid solutions, and that is why these alloys are usually referred to as medium entropy (alloys with three or four principal elements) or high entropy (alloys with at least five principal elements) alloys [3, 4].

Because high entropy alloys (HEAs) contain several principal elements, the composition domain from which an alloy can be selected is vast. Therefore, the exploration of the whole composition domain to identify alloys with desired properties is very challenging. To overcome this problem, many research works have focused on developing models for predicting the microstructure or properties of HEAs [5–9]. Such models can facilitate the exploration of the whole composition domain leading to the identification of HEAs with desired properties. Different strategies have been used to predict HEAs’ microstructure or properties [5–9]. Most of the approaches are based on thermodynamic simulations or ab initio calculations. Although these approaches successfully predicted the structure or mechanical properties of HEAs, they have limitations.

The most comprehensive model, usually used for estimating the solid solution hardening in HEAs, is the model derived by Varvenne et al. [9]. In the developed model by Varvenne et al., each elemental alloy component was assumed as a solute embedded in an adequate solvent [9]. The solute was then considered a local concentration fluctuation which can interact with dislocations leading to the hardening of the alloy [9]. Although the model has been successfully used in several research works for predicting the strength of solid-solution high entropy alloys, the theory
has some significant drawbacks, as stressed in [10]. Furthermore, it has been reported very recently that Varvenne’s model (used in a reduced form) fails to predict the changes of strength in solid solution high entropy alloys $(\text{AuNiPdPt})_{1-x}\text{Cu}_x$ [10]. Therefore, it may be concluded that a model which can accurately predict the strength of high entropy alloys is still lacking.

The present work aims to introduce a new approach to modeling the mechanical properties of solid solution HEAs. Although the introduced approach (data-based modeling and fitting) does not explain the parameters and mechanisms involved in strengthening HEAs, it can be considered a straightforward method for assessing the strength of solid solution HEAs. Therefore, the proposed approach is a valuable tool for designing HEAs. Quaternary and quinary fcc solid solution HEAs in the Co-Cr-Fe-Mn-Ni (Canty alloy-based system) are investigated in the present work. However, it is believed that the approach can also be used for other solid solution systems.

1. Methodology.

1.1. Experimental Data. The experimental dataset, shown in Table 1, is used in the present work. The data in Table 1 are gathered from a recently published paper by Bracq et al. [11]. It was reported that all of the alloys listed in Table 1 have a single-phase fcc solid solution after annealing [11] except alloy #1, which contained small amounts (4% volume fraction) of a bcc phase. Because nanoindentation tests were performed on the center of single grains, the role of grain-boundary strengthening on hardness values can be ignored. So, the hardness values can be directly attributed to the frictional stress (or the intrinsic lattice resistance to dislocation motion) and the strengthening contribution from solid solution hardening [9–12]. It should be noted that the frictional stress and solid solution hardening can be considered a chemical composition function [9–12]. Furthermore, it should be noted that because the same procedures (casting and heat treatment) were used for the preparation of alloys in Table 1, the microstructure’s role in the hardness values can be ignored, and the hardness values can be directly attributed to chemical compositions. The composition domain covered by alloys in Table 1 is schematically shown in Fig. 1. It can be seen that the dataset in Table 1 covers a noticeable part of the composition domain.

| Alloy | Chemical composition (at.%) | Hardness H (GPa) | Lattice parameter $a$ (Å) |
|-------|----------------------------|------------------|---------------------------|
|       | Co | Cr | Fe | Mn | Ni |                 |                 |
| 1     | 0  | 23.8 | 24.9 | 25.8 | 25.5 | 2.12 | 3.622 |
| 2     | 10 | 23.1 | 22.5 | 22.5 | 21.9 | 2.5 | 3.609 |
| 3     | 20 | 20.3 | 20 | 20.3 | 19.4 | 2.52 | 3.601 |
| 4     | 29.7 | 18.1 | 17.5 | 17.7 | 17 | 2.53 | 3.593 |
| 5     | 49.6 | 12.8 | 12.5 | 12.7 | 12.4 | 2.74 | 3.576 |
| 6     | 25.1 | 0 | 25 | 25.2 | 24.7 | 2.07 | 3.603 |
| 7     | 23.7 | 5.2 | 23.9 | 24.2 | 23 | 2.41 | 3.602 |
| 8     | 21.2 | 15.3 | 21.3 | 21.6 | 20.6 | 2.53 | 3.601 |
| 9     | 18.7 | 25.5 | 18.7 | 18.9 | 18.2 | 2.5 | 3.605 |
| 10    | 24.9 | 23.6 | 0 | 25.1 | 24.4 | 3.22 | 3.616 |
| 11    | 22.3 | 23 | 10 | 22.8 | 21.9 | 2.85 | 3.609 |
| 12    | 17.4 | 18.1 | 29.8 | 17.7 | 17 | 2.41 | 3.601 |
| 13    | 12.7 | 13 | 49.5 | 12.6 | 12.2 | 1.94 | 3.593 |
| 14    | 24.9 | 25.5 | 25.1 | 0 | 24.5 | 2.37 | 3.575 |
| 15    | 22.4 | 23 | 22.6 | 10.2 | 21.8 | 2.55 | 3.594 |
| 16    | 17.4 | 17.9 | 17.4 | 30.3 | 17 | 2.46 | 3.616 |
| 17    | 12.6 | 12.3 | 12.7 | 50.2 | 12.2 | 2.31 | 3.644 |
| 18    | 10.4 | 10.5 | 10.4 | 9.6 | 59.1 | 2.94 | 3.579 |
| 19    | 2.1 | 2.1 | 2.2 | 2.4 | 91.2 | 1.99 | 3.539 |
1.2. Proposed Approach. For explaining the approach, solid-solution binary systems can be considered first. For example, a Cu-Ni system with complete solid solubility can be considered. Figure 2 shows the yield stress of Cu-Ni solid solution alloys versus composition [13]. It can be seen that the yield stress ($\sigma_y$) of solid solution Cu-Ni alloys can be modeled by a polynomial where the polynomial equation can be written as follows

$$
\sigma_y = 4.449 \times Ni - 0.0321 \times Ni^2 + 0.0064 \times Cu^2,
$$

where Ni and Cu show the atomic concentration (at.%) of nickel and copper respectively.

Similarly, it can be shown that the strength of binary systems with complete solid solubilities such as Nb-Ta [14], Mo-Ta [15], or Mo-W [15] can be modeled by polynomials. Furthermore, it may be assumed that the strength of solid-solution HEAs can also be modeled by polynomials. Therefore, it is proposed in the present work that the hardness ($H$) of solid solution HEAs in the Co-Cr-Fe-Mn-Ni system can be modeled by the following polynomial:

$$
H = \sum_{i=1}^{5} (a_iC_i + b_iC_i^2),
$$

where $a_i$ and $b_i$ are coefficients to be determined and the $C_i$ is the atomic fraction of element $i$. For determining the coefficients, the above equation can be fitted to the experimental dataset in Table 1 by using the least-square method. The obtained values for coefficients are shown in Table 2.
TABLE 2. The Values of Coefficients for the Proposed Polynomial

| Element | Co | Cr | Fe | Mn | Ni |
|---------|----|----|----|----|----|
| $a_1$   | 3.5928 | 7.8797 | -2.2453 | 2.4492 | 5.5452 |
| $b_1$   | -1.9858 | -18.1814 | 4.1906 | -1.8303 | -3.9653 |

2. Results and Discussion. The comparison between the experimental data in Table 1 and the predicted results in Fig. 3 shows their good agreement, implying that the proposed equation could model the hardness of quaternary and quinary fcc solid solution alloys in the Co-Cr-Fe-Mn-Ni system.

To further evaluate the extrapolating ability of the developed polynomial, it is used for predicting the strength of some non-equiatomic alloys in the Co-Cr-Fe-Mn-Ni system. The investigated alloys are Co$_{50-x}$Cr$_{25}$Ni$_{25}$ (x = 20, 25, 30, 35) [16], Cr$_{x}$Mn$_{x}$Fe$_{25}$Co$_{3}$Ni$_{100-4x}$ (x = 2, 3, 4, 7.5, 10, 12.5, 15, 17.5, 18.75, 20) [12], Fe$_{64-x}$Mn$_{2}$Ni$_{28}$Co$_{5.6}$Cr$_{2.4}$ (x = 21, 24, 27, 34, 38) [17], Fe$_{x}$(CoCrMnNi)$_{100-x}$ (x = 20, 40, 50, 60) [18], Fe$_{x}$(NiCrCo)$_{100-x}$ (x = 25, 45, 55) [19], and CoCrFeMn$_{2}$Ni$_{2-x}$ (x = 0.25–1.25) [20]. The comparison between prediction and experimental results is shown in Fig. 4.

It can be seen that the developed polynomial can predict the changes in strength versus composition relatively well. Surprisingly, the prediction results for Cr$_{x}$Mn$_{x}$Fe$_{25}$Co$_{3}$Ni$_{100-4x}$ indicate a maximum hardness with the variation of x in good agreement with experimental results [12]. For Fe$_{64-x}$Mn$_{2}$Ni$_{28}$Co$_{5.6}$Cr$_{2.4}$ [17] and CoCrFeMn$_{2}$Ni$_{2-x}$ [20] alloy systems, small changes in hardness versus composition are predicted by the plateau observed for the strength of these alloys [17, 20]. One point which needs to be emphasized is that the relation between the yield stress and nanohardness (GPa) is not necessarily linear [21, 22]. In other words, the correlation between nanohardness and yield stress may not be linear [21, 22]. This might be the reason for the discrepancies observed in Fig. 4. According to the results in Fig. 4, it can be concluded that the developed polynomial is reliable for predicting the strength of quaternary and quinary solid solution alloys in the Co-Cr-Fe-Mn-Ni system.

Fig. 3. Comparison between the experimental results and predictions.

Fig. 4. Comparison of predicted nanohardness and yield strength with experimental data for different alloys.
Because the experimental dataset only includes quaternary and quinary alloys, the polynomial probably needs to be more accurate for binary and ternary subsystems. In other words, when the concentration of two or three elements simultaneously reaches zero, some degree of error should be expected in the prediction results. To investigate this point, experimental data in Table 3 can be considered. As can be seen, predictions show that the hardness of NiCo is higher than the hardness of alloys NiFe, NiFe-20Cr, and NiCoFe, which is different from the experimental results. So the polynomial is not valid for predicting the strength of binary systems. If empirical data can be provided for binary and ternary systems, then the polynomial can be improved for predicting the strength of binary and ternary systems.

The developed polynomial can be used to investigate the strength of quaternary and quinary alloys in the Co-Cr-Fe-Mn-Ni system. Figure 5 shows the predicted results for quaternary alloys (CoCrMn)xNi100–x, (CoCrFe)xNi100–x, (CoFeMn)xNi100–x and (CrFeMn)xNi100–x. As can be seen, the hardest alloy in each system has non-equatomic element ratios similar to the experimental results for alloy system (CoCrFeMn)xNi100–x [12]. Furthermore, it can be seen that the hardness of equiatomic alloys decreases in the following order: CoCrMnNi (3.24 GPa) > CoCrFeNi (2.44 GPa) > CrFeMnNi (3.24 GPa) > CoMnFeNi (2.44 GPa) which is in agreement to the experimental results [24] for the yield stresses: CoCrMnNi (σy = 282 MPa) > CoCrFeNi (σy = 274 MPa) > CoMnFeNi (σy = 176 MPa). These results again confirm the developed polynomial’s ability to predict the strength of HEAs.

| Alloy           | H (GPa) [23] (experiment) | H(GPa) (prediction) |
|-----------------|----------------------------|---------------------|
| NiFe-20Cr       | 1.91                       | 2.20                |
| NiCoFe          | 1.82                       | 2.11                |
| NiCoCr          | 2.74                       | (3.01)*             |
| NiCo            | 1.31                       | 3.08                |
| NiFe            | 1.96                       | 1.70                |
| Ni              | 1.18                       | 1.57                |

* The polynomial could not be used for alloy CoCrNi because the Cr concentration of this alloy is not within the Cr concentration of the dataset in Table 1.
The developed polynomial can be used to investigate constituent elements’ effect on the strength of solid solution alloys. In this regard, a MATLAB code is written (Appendix A), and more than 14000 quinary alloys are designed in the Co-Cr-Fe-Mn-Ni system. The concentration of constituent elements in designed alloys are selected in the following range: $10 < \text{Co} < 50$, $10 < \text{Cr} < 25$, $10 < \text{Fe} < 50$, $10 < \text{Mn} < 50$, and $15 < \text{Ni} < 60$. The minimum concentration of Co, Cr, Fe, and Mn is 10 at.% according to the chemical range proposed for HEAs [12]. Furthermore, the minimum concentration of Ni in designed alloys (15 at.%) is selected to be within the composition domain covered by the experimental dataset (Fig. 1).

Figure 6 shows the effect of constituent elements on the hardness of designed quinary alloys. According to the prediction results, it can be seen that by increasing the Fe content, the hardness decreases. The results in Fig. 6 suggest that the concentration of Fe should be reduced for designing harder fcc solid solution alloys in the Co-Cr-Fe-Mn-Ni system. In fact, experimental results for alloys $\text{Co}_{x}\text{Fe}_{50-x}\text{Cr}_{25}\text{Ni}_{25}$ [16], $\text{Fe}_{x}(\text{CoCrMnNi})_{100-x}$ [18] and $\text{Fe}_{x}(\text{NiCrCo})_{100-x}$ [19] indicate that strength decreases with increasing the Fe content. Furthermore, experimental results [24] indicate that Fe-free equiatomic alloy CoCrMnNi has higher yield stress than Fe-containing equiatomic alloys CoCrFeMnNi, CoFeMnNi, and CoCrFeNi [24].

It should be noted that the trends which are observed in Fig. 6 are only valid for the quinary alloy system Co-Cr-Fe-Mn-Ni and within the investigated composition domain. The effect of Fe can change with changing the alloy system or the alloy concentration. For example, it is well known that the strength will increase when Fe is added to Ni. Therefore, Fe’s strengthening or softening effect depends on the alloy system and the composition range being investigated.
Some of the important parameters which can affect the strength of a solid solution alloy are Peierls-Nabarro (PN) stress [25–28], valence electron concentration [29], atomic size differences [30], lattice distortion [21], electronegativity differences [31], elastic misfits [10], short-range orders [32], magnetism [33] and stacking fault energies [34]. Therefore, all of the above-mentioned parameters should be considered to investigate the effect of an alloying element. The trends observed for the constituent elements may be explained by considering the role of a constituent element in changing the above parameters and how changing the above parameters can affect the strength (strengthening or softening).

The effect of Fe on the hardness may be explained by considering its effect on the Peierls-Nabarro (PN) stress or the intrinsic lattice resistance to dislocation motions [18, 25–28]. Several research works have suggested that high yield stresses of solid solution HEAs are due to the enhanced PN stress of these alloys [25–28]. The PN stress for an edge dislocation can be written as

\[
\sigma_{PN} = \frac{2G}{1-\nu} \exp(-2\alpha\xi/b),
\]

where \(G\) is the shear modulus, \(\nu\) is the Poisson ratio, and \(\alpha = \xi/b\), where \(\xi\) is the dislocation core width, and \(b\) is the Burgers vector. The parameter \(\alpha\) defines the core structure of a dislocation. According to the above equation, the PN stress depends on the interatomic bonds between atoms \((G\) and \(\nu\)) and the lattice \((\alpha)\). Furthermore, it can be seen that the PN stress (and, as a result, \(H\)) decreases with the decreasing shear modulus \((G)\). It was reported that Fe-containing solid solution alloys generally have lower elastic constants [12, 30]. Furthermore, following elastic constants are proposed for constituent elements in Co-Cr-Fe-Mn-Ni system: \(G_{Co} = 81\) GPa, \(G_{Cr} = 103.5\) GPa, \(G_{Fe} = 51.7\) GPa, \(G_{Mn} = 81\) GPa, \(G_{Ni} = 76\) GPa [12, 30]. It can be seen that Fe has the lowest elastic modulus among the constituent elements. Therefore, it can be predicted that the shear modulus and, as a result, the PN stress will decrease with the addition of Fe. This may be the reason for decreasing the strength with increasing the Fe content of quinary alloys.

The hardest quinary alloy in the Co-Cr-Fe-Mn-Ni system within the investigated composition range is predicted to be \(\text{Co}_{28}\text{Cr}_{14}\text{Fe}_{10}\text{Mn}_{10}\text{Ni}_{38}\) with a hardness of 3.17 GPa. Furthermore, the softest quinary alloy within the analyzed composition range is expected to be \(\text{Co}_{10}\text{Cr}_{20}\text{Fe}_{40}\text{Mn}_{10}\text{Ni}_{14}\) with a hardness of 1.85 GPa. This example shows how the developed polynomial could identify the softest or hardest alloy in the Co-Cr-Fe-Mn-Ni system. A similar approach also could be used for quaternary systems. Therefore, the developed polynomial can be considered a convenient tool for designing HEAs.

It was proposed that parameters such as lattice distortion, atomic size difference, valence electron concentration, elastic moduli, dislocation widths, and electronegativity difference could affect the strength of solid solution HEAs [1–4]. The developed model can assess the relationship between these parameters and the strength of
solid solution HEAs in Co-Cr-Fe-Mn-Ni. The relation between parameters enthalpy of mixing ($\Delta H_{mix}$) and valence electron concentration (VEC) and the strength of alloys is investigated here. These parameters are selected here because their effects on the strength of solid solution alloys are not well studied. The impact of enthalpy of mixing ($\Delta H_{mix}$) on the microstructure of HEAs is well studied [3, 4], but the effect of $\Delta H_{mix}$ on the strength of HEAs is not inspected so far. So, for the first time, the effect of $\Delta H_{mix}$ on the strength of HEAs was investigated. Mixing enthalpy ($\Delta H_{mix}$) can be regarded as the result of interactions between the constituent elements [35], so it is reasonable to assume that $\Delta H_{mix}$ can affect the strength of atomic bonds and the mechanical behavior of an alloy. The enthalpy of mixing ($\Delta H_{mix}$) for alloys can be estimated by the following equation [3, 4]:

$$\Delta H_{mix} = \sum_{i=1,i\neq j}^{n} (4\Delta H_{AB}^{mix})C_iC_j,$$

(4)

where $\Delta H_{AB}^{mix}$ is the mixing enthalpy of binary liquid alloys and the values can be obtained from [36], $C_i$ is the atomic fraction of element $i$, and $C_j$ is the atomic fraction of element $j$. The relationship between $H$ and $\Delta H_{mix}$ for designed alloys is shown in Fig. 7.

![Fig. 7. The relation between the enthalpy of mixing ($\Delta H_{mix}$) and the hardness ($H$) of designed quinary HEAs in the Co-Cr-Fe-Mn-Ni system.](image)

According to this figure, a correlation between $\Delta H_{mix}$ and $H$ can be seen, and $H$ increases with the decreasing value of $\Delta H_{mix}$. So it can be concluded that $\Delta H_{mix}$ has essential effects on the strength of HEAs and can be considered a guideline for designing stronger HEAs. In other words, $\Delta H_{mix}$ should be more negative to create stronger solid-solution fcc HEAs. For example, one may name fcc single solid solution equiatomic CoNiV alloy [37]. This alloy’s room temperature yield stress is reported to be 688 MPa (grain size of 8 μm) [37], much higher than the yield stress of fcc solid solution alloys in the Co-Cr-Fe-Mn-Ni system. On the other hand, $\Delta H_{mix}$ for CoNiV alloy is -14.2 kJ/mol, which is much more negative than the $\Delta H_{mix}$ for fcc solid solution alloys in the Co-Cr-Fe-Mn-Ni system. So outstanding yield strength of CoNiV alloy may be attributed to its more negative $\Delta H_{mix}$, according to Fig. 7. As another example, one may name fcc single solid solution alloy Ni$_{63.2}$V$_{36.8}$ [31] with excellent room temperature yield stress of 750 MPa (grain size of 8 μm), which is again much higher than the yield stress of fcc solid solution alloys in Co-Cr-Fe-Mn-Ni system. The $\Delta H_{mix}$ for this alloy is -16.745 kJ/mol, which is much more harmful than the $\Delta H_{mix}$ for alloys in the Co-Cr-Fe-Mn-Ni system.

According to the classical model by Miedema [38], more negative values of enthalpy of mixing are due to the increased hybridization because of the larger charge sharing between the atoms [38]. In other words, more negative values of enthalpy of mixing indicate stronger atomic bonds between the constituent elements (and probably higher elastic modules), which may explain the observed relationships in Fig. 7. Furthermore, very recently, Oh et al. [31] have shown that the governing parameter for solid-solution strengthening in single-phase fcc HEAs consisting of 3d
transition metal elements is the variation in the atomic-level pressures originating from the charge transfer between neighboring elements [31]. So, considering the effect of charge transfer on the enthalpy of mixing, the relationships observed in Fig. 7 may also be explained [31, 38]. In other words, more charge transfer causes more atomic-level pressures leading to stronger alloys, according to [31]. On the other hand, more amount of charge transfer leads to more negative values of enthalpy of mixing according to Miedema’s model, and this might be the reason for the relationships observed in Fig. 7.

The observed relation between hardness and enthalpy of mixing can also be explained by considering the presence of short-range chemical order (SRO) in solid solution high entropy alloys. It has been shown that the distribution of elements in solid solution HEAs is not entirely random, and short-range chemical order (SRO) exists in the structure of these alloys [39–43]. Furthermore, direct atomistic simulations predict that SRO has a negative contribution to the heat of mixing in the order of meV/atom [40–43]. Therefore, with increasing the extent of SRO, the enthalpy of mixing decreases, and more heat is released during the solution formation. On the other hand, the presence of SRO can increase the lattice resistance to dislocation motions leading to the hardening of the alloy [44, 45]. So, it can be speculated that solid solutions with lower values of $\Delta H_{\text{mix}}$ should have a higher degree of SRO, which could be the reason for increasing the strength with decreasing enthalpy of mixing (Fig. 7).

The relation between valance electron concentration (VEC) and the hardness of designed alloys is investigated, and the results are shown in Fig. 8. The following equation is used for calculating VEC:

$$VEC = \sum_{i=1}^{5} C_i \times VEC_i,$$

where $C_i$ is the atomic fraction of element $i$ and $VEC_i$ is the valence electron concentration of element $i$ values can be found in [3]. According to Fig. 8, the hardness increases with increasing VEC for designed alloys within the investigated composition. High VEC leads to greater atomic bond forces [29], which may be why the relationship is observed in Fig. 8. Another speculation for the relation observed in Fig. 8 could be increasing the directionality of the electron bond forces with increasing valence electron concentration which can increase the PN stress of an alloy [46, 47]. Further studies are needed to explain the relationship between hardness and VEC.

Fig. 8. The relation between the valence electron concentration (VEC) and the hardness ($H$) of designed quinary HEAs in the Co-Cr-Fe-Mn-Ni system.

In the end, the developed approach may also be used for modeling other properties of solid solution alloys. For example, the proposed polynomial is applied for modeling the lattice parameter of alloys in Table 1, and the coefficients in Table 4 are obtained after fitting the polynomial to the experimental data. The comparisons between the predictions and experimental data are shown in Fig. 9, and an excellent agreement can be seen. Therefore, the approach proposed here may also be used to model other solid solution alloys’ properties.
TABLE 4. The Values of Coefficients for the Proposed Polynomial to Model the Lattice Parameter of Alloys

| Element | Co  | Cr  | Fe  | Mn  | Ni  |
|---------|-----|-----|-----|-----|-----|
| $a_i$   | 3.5346 | 3.5683 | 3.5407 | 3.7094 | 3.6359 |
| $b_i$   | -0.0017 | 0.1541 | 0.0653 | 0.0092 | -0.1118 |

Fig. 9. Comparison between the experimental results and predictions for lattice parameter.

Conclusions. A simple methodology is proposed for predicting the strength of quaternary and quinary fcc solid solution high entropy alloys in the Co-Cr-Fe-Mn-Ni system. The strength of alloys could be modeled by a second-order polynomial, with coefficients derived from the experimental data. The results show that the proposed polynomial could accurately model the hardness of solid solution alloys. The proposed polynomial only requires the element concentrations as inputs, making it very convenient to apply. The developed polynomial is used to predict the strength of quinary HEAs in the Co-Cr-Fe-Mn-Ni system. The results indicate that with increasing the Fe concentration in designed quinary alloys, the strength of alloys decreases in agreement with experiential data. The softening effect of Fe is explained by considering its effect on reducing the shear modulus and the Peierls-Nabarro stress of alloys. The impacts of enthalpy of mixing and valence electron concentration on the strength of HEAs are investigated. The results show that the enthalpy of mixing has a noticeable effect on the hardness of quinary Co-Cr-Fe-Mn-Ni alloys, and the strength of alloys increases with the decreasing mixing enthalpy. Furthermore, the results show that quinary Co-Cr-Fe-Mn-Ni alloys’ hardness increases with the parameter valence electron concentration. Explanations are made to describe the observed relationships.

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