**Supplementary Information**

**Machine learning based phase prediction and powder metallurgy assisted experimental validation of medium entropy compositionally complex alloys**

This document contains the dataset of all medium entropy alloys (MEAs) along with their mixing entropy (), mixing enthalpy (), , , atomic size mismatch (), , Pauling electronegativity () and molar volume dispersity () values. Equation 1-8 (of the manuscript) was used to calculate the above-mentioned parameters. The phase/phases of an MEA mentioned in the dataset were the experimentally determined phase/phases employing X-ray diffraction (XRD), scanning electron microscope (SEM) and transmission electron microscope (TEM). The abbreviation used for different phases are SS for solid solution, SS+IM for solid solution + intermetallic and AM for amorphous. The ordered intermetallic phase, such as the B2 phase is considered intermetallic (IM) in this work.

The alloy compositions are given in atomic percent for ease of calculation of the parameters. For instance, AaBbCcDd indicates that the elements A, B, C, D have the atomic percent of a, b, c, d, respectively. In case of equiatomic alloys i.e a = b = c = d, only ABCD is written. The notation (ABCD)T signifies T atomic percent is equally distributed among elements A, B, C and D.

**Summary of ML datasets**

**Table S1:** The dataset was used for ternary classification of phases in MEA (SS, SS+IM, AM). The dataset provides coverage of experimentally fabricated MEAs, reported in literature till November 2022.

**Table S2:** The dataset was used for binary classifications B1 (SS, SS+IM) and B2 (SSS, MSS). The dataset provides coverage of experimentally fabricated MEAs, reported in literature till November 2022.

**Table S3:** The dataset was used for phase prediction in the case study section. The dataset provides coverage of experimentally fabricated MEAs, reported in the literature between November 2022 and February 2023.

**Table S4:** The dataset was used for ternary classification of phases in HEA (SS, SS+IM, AM). The number of instances of different phases kept same as MEA dataset. The datapoints were randomly collected from [25][27][48]

**Summary of other tables**

**Table S5:** Optimized parameters for ternary phase classification in HEA dataset

**Table S6:** Optimized parameters for B1 and B2 classification

**Table S1:** Mixing entropy (), mixing enthalpy (), , , atomic size mismatch (), , Pauling electronegativity () and molar volume dispersity (), phase name and category for MEAs. Dataset used for ternary classification of phases in MEA (SS, SS+IM, AM)

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Medium entropy alloy composition** | **(J/K)** | **(KJ/mol)** |  |  |  |  |  |  | **Phase name** | **Phase category** | **Reference** |
| FeCrNiAl | 11.53 | -21.02 | 1.56 | 1.157 | 5.52 | 0.377 | 0.12 | 0.172 | BCC+B2 | SS+IM | [1] |
| Fe35(CrNiAl)65 | 11.32 | -11.5 | 1.65 | 1.157 | 5.31 | 0.4 | 0.116 | 0.164 | BCC+B2 | SS+IM | [1] |
| Fe45(CrNiAl)55 | 10.47 | -9.81 | 1.86 | 1.158 | 5.04 | 0.422 | 0.11 | 0.155 | BCC+B2 | SS+IM | [1] |
| Fe55(CrNiAl)45 | 9.83 | -8.09 | 2.09 | 1.158 | 4.70 | 0.444 | 0.101 | 0.144 | BCC+B2 | SS+IM | [1] |
| Fe65(CrNiAl)35 | 8.58 | -6.35 | 2.35 | 1.158 | 4.26 | 0.47 | 0.091 | 0.130 | BCC+B2 | SS+IM | [1] |
| CrCoNi | 9.13 | -4.28 | 4.03 | 1.034 | 1.49 | 4.099 | 0.111 | 0.041 | FCC | SS | [2] |
| FeCrNiCo | 11.53 | -3.71 | 5.80 | 1.034 | 1.29 | 6.835 | 0.096 | 0.039 | FCC | SS | [3] |
| FeCrNiMn | 11.53 | -3.83 | 5.44 | 1.104 | 3.64 | 0.867 | 0.14 | 0.040 | FCC+BCC | SS | [3] |
| FeNiCoMn | 11.53 | -3.82 | 5.14 | 1.104 | 3.95 | 0.738 | 0.142 | 0.044 | FCC | SS | [3] |
| FeCoCrMn | 11.53 | -2.29 | 9.16 | 1.104 | 3.64 | 0.867 | 0.132 | 0.036 | FCC+BCC | SS | [3] |
| NiCoCrMn | 11.53 | -5.6 | 3.69 | 1.104 | 3.79 | 0.799 | 0.15 | 0.047 | FCC | SS | [3] |
| FeNiCo | 9.13 | -1.62 | 9.97 | 1.008 | 0.37 | 64.565 | 0.032 | 0.032 | FCC | SS | [3] |
| FeNiCr | 9.13 | -4.28 | 4.06 | 1.034 | 1.34 | 5.072 | 0.104 | 0.039 | FCC | SS | [3] |
| FeNiMn | 9.13 | -4.17 | 3.69 | 1.104 | 4.20 | 0.516 | 0.154 | 0.044 | FCC | SS | [3] |
| FeCoMn | 9.13 | -2.4 | 6.46 | 1.104 | 4.20 | 0.516 | 0.145 | 0.039 | FCC+BCC | SS | [3] |
| NiCoMn | 9.13 | -5.99 | 2.55 | 1.104 | 4.38 | 0.474 | 0.163 | 0.049 | FCC | SS | [3] |
| NiCrMn | 9.13 | -5.61 | 2.94 | 1.103 | 3.82 | 0.623 | 0.15 | 0.047 | FCC | SS | [3] |
| CoCrMn | 9.13 | -3.3 | 5.03 | 1.103 | 3.82 | 0.623 | 0.137 | 0.041 | FCC++IM | SS+IM | [3] |
| WNbMoTa | 11.53 | -6.55 | 5.55 | 1.053 | 2.27 | 2.228 | 0.096 | 0.069 | BCC | SS | [4] |
| Zr66Al8Cu12Ni14 | 8.36 | -37.81 | 0.41 | 1.296 | 9.79 | 0.087 | 0.250 | 0.266 | AM | AM | [5] |
| Zr66Al9Cu16Ni9 | 8.32 | -35.15 | 0.44 | 1.296 | 9.51 | 0.091 | 0.246 | 0.26 | AM | AM | [5] |
| Zr65Al7.5Cu17.5Ni10 | 8.39 | -34.42 | 0.45 | 1.296 | 9.81 | 0.087 | 0.253 | 0.268 | AM | AM | [5] |
| La55Al25Ni15Cu5 | 9.23 | -40.93 | 0.27 | 1.533 | 16.33 | 0.034 | 0.334 | 0.431 | AM | AM | [5] |
| La55Al25Ni10Cu10 | 9.44 | -39.13 | 0.28 | 1.532 | 16.18 | 0.036 | 0.333 | 0.428 | AM | AM | [5] |
| La55Al25Ni5Cu15 | 9.23 | -37.4 | 0.29 | 1.532 | 16.04 | 0.035 | 0.333 | 0.426 | AM | AM | [5] |
| Cu54Zr27Ti9Be10 | 9.42 | -20.68 | 0.74 | 1.463 | 11.74 | 0.068 | 0.249 | 0.36 | AM | AM | [5] |
| Ti34Zr11Cu47Ni8 | 9.7 | -15.1 | 1.07 | 1.308 | 8.62 | 0.130 | 0.214 | 0.267 | AM | AM | [5] |
| Pd40Cu30Ni10P20 | 10.64 | -33.2 | 0.44 | 1.261 | 7.75 | 0.177 | 0.144 | 0.3 | AM | AM | [5] |
| Pd40Ni40P20 | 8.77 | -31.05 | 0.41 | 1.262 | 7.86 | 0.142 | 0.140 | 0.314 | AM | AM | [5] |
| Zr57Ti5Al10Cu20Ni8 | 10.18 | -34.67 | 0.53 | 1.297 | 9.68 | 0.108 | 0.249 | 0.271 | AM | AM | [5] |
| Zr38.5Ti16.5Ni9.75Cu15.25B20 | 12.47 | -51.22 | 0.59 | 2.006 | 22.26 | 0.025 | 0.296 | 0.396 | AM | AM | [5] |
| Zr39.88Ti15.12Ni9.98Cu13.77Be21.25 | 12.34 | -34.1 | 0.66 | 1.458 | 13.85 | 0.064 | 0.221 | 0.385 | AM | AM | [5] |
| Zr41.2Ti13.8Ni10Cu12.5Be22.5 | 12.18 | -35.01 | 0.63 | 1.458 | 14.08 | 0.061 | 0.219 | 0.390 | AM | AM | [5] |
| Zr42.63Ti12.37Ni10Cu11.25Be23.75 | 11.97 | -35.92 | 0.61 | 1.458 | 14.32 | 0.058 | 0.217 | 0.395 | AM | AM | [5] |
| Zr44Ti11Ni10Cu10Be25 | 11.73 | -36.82 | 0.58 | 1.458 | 14.55 | 0.055 | 0.214 | 0.4 | AM | AM | [5] |
| Zr45.38Ti9.62Ni10Cu8.75Be26.25 | 11.46 | -37.71 | 0.56 | 1.458 | 14.78 | 0.052 | 0.212 | 0.405 | AM | AM | [5] |
| Zr46.25Ti8.25Ni10.5Cu7.5Be27.5 | 11.21 | -38.77 | 0.53 | 1.458 | 15 | 0.049 | 0.210 | 0.411 | AM | AM | [5] |
| La55Al25Ni5Cu10Co5 | 10.02 | -38 | 0.31 | 1.532 | 16.16 | 0.038 | 0.331 | 0.428 | AM | AM | [5] |
| Nd60Al15Ni10Cu10Fe5 | 9.99 | -31.47 | 0.41 | 1.472 | 14.99 | 0.044 | 0.327 | 0.398 | AM | AM | [5] |
| Nd61Al11Ni8Co5Cu15 | 9.82 | -30.39 | 0.42 | 1.472 | 15.3 | 0.042 | 0.304 | 0.405 | AM | AM | [5] |
| CuFeMn | 9.13 | 7.49 | 1.90 | 1.094 | 3.67 | 0.677 | 0.151 | 0.016 | Dual FCC | SS | [6] |
| Al7.5(CuFeMn)92.5 | 10.66 | 0.75 | 21.63 | 1.147 | 4.33 | 0.568 | 0.150 | 0.101 | BCC+FCC | SS | [6] |
| Al15(CuFeMn)85 | 11.28 | -4.99 | 3.31 | 1.147 | 4.77 | 0.494 | 0.149 | 0.133 | BCC+FCC | SS | [6] |
| Fe57.5(CoNi)32.5Cr10 | 9.47 | -1.86 | 9.28 | 1.034 | 0.87 | 12.274 | 0.065 | 0.033 | FCC | SS | [7] |
| Fe60(CoNi)30Cr10 | 9.19 | -1.79 | 9.39 | 1.034 | 0.86 | 12.164 | 0.064 | 0.032 | FCC | SS | [7] |
| Fe62.5(CoNi)27.5Cr10 | 8.89 | -1.71 | 9.51 | 1.034 | 0.85 | 12.026 | 0.064 | 0.031 | FCC+BCC | SS | [7] |
| Fe60(MnCoNiCr)40 | 10.21 | -1.68 | 10.97 | 1.105 | 2.69 | 1.404 | 0.102 | 0.031 | FCC | SS | [7] |
| Fe65(MnCoNiCr)35 | 9.42 | -1.43 | 11.91 | 1.105 | 2.54 | 1.454 | 0.096 | 0.029 | FCC+HCP | SS | [7] |
| Fe70(MnCoNiCr)30 | 8.54 | -1.19 | 12.97 | 1.105 | 2.37 | 1.512 | 0.092 | 0.027 | FCC+BCC+HCP | SS | [7] |
| (CrFeNi)93.75Al6.25 | 10.51 | -9.58 | 2.02 | 1.159 | 3.35 | 0.934 | 0.110 | 0.108 | FCC | SS | [8] |
| (CrFeNi)88.2Al11.8 | 11.07 | -13.64 | 1.45 | 1.158 | 4.27 | 0.605 | 0.115 | 0.137 | FCC+BCC+B2 | SS+IM | [8] |
| (CrFeNi)83.4Al8.3Ti8.3 | 12.32 | -16.36 | 1.37 | 1.194 | 5.43 | 0.416 | 0.113 | 0.17 | FCC+BCC+B2 | SS+IM | [8] |
| (CrFeNi)83.4Al11.1Ti5.5 | 12.24 | -16.75 | 1.31 | 1.194 | 5.25 | 0.443 | 0.115 | 0.165 | FCC+BCC+B2 | SS+IM | [8] |
| Co17.5Cr12.5Fe55Ni10Mo5 | 10.59 | -2.21 | 9.06 | 1.132 | 2.56 | 1.612 | 0.099 | 0.079 | FCC | SS | [9] |
| Co18Cr12.5Fe55Ni7Mo7.5 | 10.62 | -2.23 | 3.17 | 1.132 | 3.01 | 1.169 | 0.111 | 0.092 | FCC | SS | [9] |
| TiZrHf | 9.13 | -0.12 | 164.9 | 1.095 | 3.80 | 0.631 | 0.106 | 0.116 | HCP | SS | [10] |
| Ti40Zr20Hf10Nb20Ta10 | 12.23 | 2.07 | 13.79 | 1.096 | 3.85 | 0.823 | 0.109 | 0.122 | BCC | SS | [10] |
| (CrCoNi)96.78Si3.22 | 10.02 | -8.76 | 2.15 | 1.099 | 1.87 | 2.840 | 0.110 | 0.137 | FCC | SS | [11] |
| (CrCoNi)93.75Si6.25 | 10.51 | -12.03 | 1.64 | 1.099 | 2.16 | 2.246 | 0.109 | 0.180 | FCC | SS | [11] |
| (CrCoNi)90.9Si9.1 | 10.84 | -14.89 | 1.36 | 1.1 | 2.38 | 1.904 | 0.108 | 0.208 | FCC | SS | [11] |
| Ti45(AlCrNb)55 | 10.74 | -22.84 | 0.91 | 1.148 | 4.74 | 0.476 | 0.045 | 0.131 | BCC+IM | SS+IM | [12] |
| Ti50(AlCrNb)50 | 10.33 | -21.65 | 0.92 | 1.148 | 4.58 | 0.490 | 0.045 | 0.126 | BCC+IM | SS+IM | [12] |
| Ti55(AlCrNb)45 | 9.83 | -20.29 | 0.94 | 1.148 | 4.40 | 0.506 | 0.045 | 0.120 | BCC+IM | SS+IM | [12] |
| Ti60(AlCrNb)40 | 9.25 | -18.75 | 0.96 | 1.148 | 4.20 | 0.522 | 0.044 | 0.114 | BCC | SS | [12] |
| Ti65(AlCrNb)35 | 8.58 | -17.03 | 0.98 | 1.147 | 3.98 | 0.541 | 0.042 | 0.107 | BCC | SS | [12] |
| Ti27V33Ta40 | 9.03 | -0.52 | 44.44 | 1.095 | 3.94 | 0.580 | 0.055 | 0.115 | BCC | SS | [13] |
| Ti33V33Ta34 | 9.13 | -0.55 | 41.34 | 1.095 | 3.94 | 0.586 | 0.054 | 0.115 | BCC | SS | [13] |
| Ti40V33Ta27 | 9.03 | -0.63 | 34.15 | 1.095 | 3.94 | 0.580 | 0.052 | 0.114 | BCC | SS | [13] |
| Ti45V20Ta35 | 8.72 | 0 | 14119 | 1.095 | 3.31 | 0.791 | 0.046 | 0.094 | BCC | SS | [13] |
| Ni57.6Cr19.2Fe19.2Nb4 | 8.98 | -7.25 | 2.31 | 1.196 | 3.45 | 0.751 | 0.106 | 0.119 | FCC | SS | [14] |
| TiZrNbTa | 11.53 | 2.46 | 11.82 | 1.096 | 3.74 | 0.821 | 0.1 | 0.121 | BCC | SS | [15] |
| Al7.5(CoCrNi)92.5 | 10.66 | -11.88 | 1.63 | 1.159 | 3.72 | 0.769 | 0.120 | 0.124 | FCC | SS | [16] |
| (CoCrNi)96.8Mo3.2 | 10.02 | -5.2 | 3.71 | 1.132 | 2.40 | 1.737 | 0.125 | 0.076 | FCC | SS | [17] |
| (CoCrNi)93.75Mo6.25 | 10.51 | -5.34 | 3.84 | 1.132 | 2.97 | 1.190 | 0.136 | 0.096 | FCC | SS | [17] |
| Fe50(CoCrMnNi)50 | 11.53 | -2.22 | 9.38 | 1.105 | 2.96 | 1.314 | 0.113 | 0.034 | FCC | SS | [18] |
| (CoCrNi)99W1 | 9.51 | -4.97 | 3.65 | 1.141 | 1.87 | 2.692 | 0.111 | 0.056 | FCC | SS | [19] |
| (CoCrNi)98W2 | 9.77 | -4.92 | 3.82 | 1.141 | 2.19 | 2.033 | 0.111 | 0.067 | FCC | SS | [19] |
| (CoCrNi)97W3 | 9.98 | -4.87 | 3.99 | 1.141 | 2.45 | 1.652 | 0.111 | 0.076 | FCC | SS | [19] |
| (CoFeNi)96.8Al3.2 | 10.02 | -4.43 | 3.94 | 1.160 | 2.50 | 1.595 | 0.056 | 0.088 | FCC | SS | [20] |
| (CoFeNi)88.2Al11.8 | 11.07 | -12.32 | 1.50 | 1.159 | 4.48 | 0.551 | 0.090 | 0.147 | FCC+B2/BCC | SS+IM | [20] |
| (CoFeNi)83.3Al16.7 | 11.36 | -16.62 | 1.14 | 1.158 | 5.14 | 0.429 | 0.102 | 0.166 | FCC+B2/BCC | SS+IM | [20] |
| (CoFeNi)88.2Ti11.8 | 11.07 | -11.68 | 1.69 | 1.195 | 5.46 | 0.37 | 0.111 | 0.174 | FCC+BCC | SS | [20] |
| Ni47.5Cr23.75Co23.75Ti5 | 9.86 | -9.01 | 2.03 | 1.196 | 3.83 | 0.668 | 0.121 | 0.126 | FCC | SS | [21] |
| Fe50Mn25Ni10Cr15 | 10.04 | -1.49 | 12.05 | 1.104 | 3.64 | 0.757 | 0.13 | 0.029 | FCC | SS | [22] |
| Fe48.5Mn24.25Ni9.7Cr14.55Al3 | 10.86 | -4.24 | 4.51 | 1.158 | 4.01 | 0.673 | 0.13 | 0.073 | FCC | SS | [22] |
| Fe47.5Mn23.75Ni9.5Cr14.25Al5 | 11.19 | -5.98 | 3.26 | 1.158 | 4.23 | 0.625 | 0.13 | 0.090 | FCC+BCC | SS | [22] |
| Fe47Mn23.5Ni9.4Cr14.1Al6 | 11.33 | -6.81 | 2.88 | 1.157 | 4.33 | 0.604 | 0.129 | 0.097 | FCC+BCC | SS | [22] |
| Fe46.5Mn23.25Ni9.3Cr13.95Al7 | 11.45 | -7.64 | 2.58 | 1.157 | 4.42 | 0.584 | 0.129 | 0.103 | FCC+BCC | SS | [22] |
| Fe46Mn23Ni9.2Cr13.8Al8 | 11.56 | -8.44 | 2.35 | 1.157 | 4.51 | 0.567 | 0.129 | 0.109 | FCC+BCC | SS | [22] |
| (AlCr)33.4 Fe33.3Ni33.3 | 11.05 | -16.78 | 1.11 | 1.158 | 4.96 | 0.448 | 0.116 | 0.158 | FCC+BCC+B2 | SS+IM | [23] |
| Ni46Cr23Fe23Al4Ti4 | 10.73 | -11.36 | 1.72 | 1.195 | 4.19 | 0.610 | 0.111 | 0.136 | FCC+L12 | SS+IM | [24] |
| Ni50Cr25Co25 | 8.64 | -4.46 | 1.37 | 1.034 | 1.37 | 4.574 | 0.104 | 0.039 | FCC | SS | [24] |
| Fe40Co40Ni10Al10 | 9.92 | -10.04 | 1.67 | 1.159 | 4.15 | 0.574 | 0.08 | 0.135 | BCC+FCC | SS | [25] |
| Fe40Co40Ni10Mn10 | 9.92 | -1.74 | 10.01 | 1.105 | 2.76 | 1.299 | 0.097 | 0.037 | BCC+FCC | SS | [25] |
| Co38Cr33Ni29 | 9.08 | -3.95 | 4.35 | 1.034 | 1.48 | 4.097 | 0.110 | 0.041 | FCC | SS | [26] |
| Co42Cr33Ni25 | 8.95 | -3.64 | 4.65 | 1.034 | 1.48 | 4.038 | 0.109 | 0.040 | FCC | SS | [26] |
| Hf20Nb10Ti35Zr35 | 10.7 | 1.01 | 23.2 | 1.095 | 4.09 | 0.639 | 0.118 | 0.126 | BCC | SS | [27] |
| Fe7.7(CrNiAl)92.3 | 10.69 | -15.96 | 1.09 | 1.156 | 5.76 | 0.321 | 0.129 | 0.182 | BCC+B2 | SS+IM | [28] |
| VCoNi | 9.13 | -14.79 | 1.16 | 1.086 | 3.67 | 0.676 | 0.125 | 0.110 | FCC | SS | [29] |
| Ti60Mo10V10Cr10Zr10 | 10.21 | -3.97 | 5.40 | 1.260 | 5.48 | 0.339 | 0.203 | 0.164 | BCC | SS | [30] |
| (CoCrNi)98.95Ce1.05 | 9.52 | -5.36 | 3.34 | 1.552 | 4.78 | 0.415 | 0.131 | 0.206 | FCC | SS | [31] |
| (CoCrNi)97.39Ce2.61 | 9.9 | -5.84 | 3.17 | 1.155 | 7.21 | 0.19 | 0.156 | 0.309 | FCC+HCP | SS | [31] |
| (CoCrNi)95.8Ce4.2 | 10.2 | -6.31 | 3.00 | 1.549 | 8.94 | 0.127 | 0.177 | 0.376 | AM | AM | [31] |
| (CoCrNi)94.04Ce5.96 | 10.47 | -6.81 | 2.83 | 1.547 | 10.43 | 0.096 | 0.197 | 0.430 | AM | AM | [31] |
| (CoCrNi)96.8Zr3.2 | 10.02 | -8.82 | 2.15 | 1.319 | 4.88 | 0.419 | 0.139 | 0.184 | FCC | SS | [32] |
| (CoCrNi)93.7Zr6.3 | 10.51 | -12.15 | 1.64 | 1.318 | 6.50 | 0.248 | 0.159 | 0.242 | FCC+HCP | SS | [32] |
| (CoCrNi)90.9Zr9.1 | 10.84 | -15.06 | 1.37 | 1.317 | 7.60 | 0.187 | 0.175 | 0.278 | FCC+HCP | SS | [32] |
| Ti44V44Cr9Al3 | 8.68 | -6.53 | 2.71 | 1.15 | 4.72 | 0.389 | 0.047 | 0.136 | BCC | SS | [33] |
| Ti44V44Cr6Al6 | 8.81 | -9.67 | 1.82 | 1.149 | 4.51 | 0.432 | 0.046 | 0.130 | BCC | SS | [33] |
| Ti44V44Cr3Al9 | 8.68 | -12.67 | 1.34 | 1.149 | 4.28 | 0.473 | 0.044 | 0.123 | BCC | SS | [33] |
| Al9.1(CrFeNi)90.9 | 10.84 | -11.47 | 1.67 | 1.158 | 3.87 | 0.721 | 0.113 | 0.125 | FCC+BCC | SS | [34] |
| Al10.4(CrFeNi)89.6 | 10.96 | -12.72 | 1.55 | 1.158 | 4.08 | 0.655 | 0.114 | 0.132 | FCC+BCC | SS | [34] |
| Al11(CrFeNi)89 | 11.01 | -13.09 | 1.51 | 1.158 | 4.16 | 0.634 | 0.114 | 0.134 | FCC+BCC+B2 | SS+IM | [34] |
| Al14.3(CrFeNi)85.7 | 11.24 | -15.3 | 1.29 | 1.158 | 4.59 | 0.532 | 0.117 | 0.147 | BCC+B2 | SS+IM | [34] |
| AgCuAl | 9.13 | -6.34 | 1.69 | 1.134 | 5.29 | 0.326 | 0.144 | 0.156 | FCC | SS | [35] |
| Ti35Zr15Ta25Nb25 | 11.18 | 2.14 | 13.11 | 1.096 | 3.11 | 1.151 | 0.084 | 0.104 | BCC | SS | [36] |
| Al50(TiCrMnV)50 | 11.53 | -30.33 | 0.54 | 1.15 | 3.91 | 0.753 | 0.036 | 0.137 | BCC+FCC | SS | [37] |
| Al50Ti20Cr20Mn10 | 10.15 | -31.81 | 0.46 | 1.149 | 4.46 | 0.509 | 0.041 | 0.145 | FCC+BCC+IM | SS+IM | [37] |
| Al50Ti20Cr15Mn15 | 10.29 | -32.71 | 0.44 | 1.149 | 4.08 | 0.615 | 0.040 | 0.144 | FCC+BCC+IM | SS+IM | [37] |
| Al50Ti20Cr10Mn20 | 10.15 | -33.64 | 0.41 | 1.149 | 3.66 | 0.756 | 0.038 | 0.143 | FCC+BCC+IM | SS+IM | [37] |
| Al50Ti25Cr15Mn10 | 10.04 | -33.96 | 0.42 | 1.149 | 4.13 | 0.587 | 0.041 | 0.136 | FCC+BCC+IM | SS+IM | [37] |
| Al50Ti15Cr15Mn20 | 10.29 | -31.29 | 0.45 | 1.149 | 4.01 | 0.638 | 0.04 | 0.150 | FCC+BCC+IM | SS+IM | [37] |
| Al50Ti15Cr15Mn15V5 | 11.22 | -31.02 | 0.51 | 1.149 | 4.06 | 0.677 | 0.039 | 0.144 | FCC+BCC+IM | SS+IM | [37] |
| Al50(TiCrMn)37.5V12.5 | 11.53 | -30.33 | 0.54 | 1.15 | 3.91 | 0.753 | 0.036 | 0.137 | FCC+BCC+IM | SS+IM | [37] |
| Al50(TiCrMn)30V20 | 11.3 | -29.65 | 0.55 | 1.150 | 3.74 | 0.807 | 0.034 | 0.129 | FCC+BCC+IM | SS+IM | [37] |
| Ti60Al6(VCrNb)34 | 10.11 | -10.36 | 1.97 | 1.148 | 4.45 | 0.509 | 0.045 | 0.123 | BCC | SS | [38] |
| Ti60Al8(VCrNb)32 | 10.18 | -12.66 | 1.60 | 1.148 | 4.34 | 0.540 | 0.044 | 0.119 | BCC | SS | [38] |
| Ti60Al10(VCrNb)30 | 10.21 | -14.89 | 1.34 | 1.148 | 4.22 | 0.571 | 0.044 | 0.116 | BCC | SS | [38] |
| Ti60Al12(VCrNb)28 | 10.18 | -17.04 | 1.15 | 1.148 | 4.10 | 0.603 | 0.043 | 0.112 | BCC+B2 | SS+IM | [38] |
| Ti60Al18(VCrNb)22 | 9.89 | -23.01 | 0.79 | 1.148 | 3.71 | 0.716 | 0.041 | 0.101 | BCC+B2 | SS+IM | [38] |
| TiZrNb | 9.13 | 2.53 | 8.19 | 1.096 | 4.09 | 0.556 | 0.115 | 0.131 | BCC | SS | [39] |
| Fe61Mn18Si11Cr10 | 9.01 | -12.33 | 1.30 | 1.174 | 4.13 | 0.526 | 0.118 | 0.199 | BCC+FCC | SS | [40] |
| HfNbTa | 9.13 | 3.00 | 8.67 | 1.088 | 3.74 | 0.650 | 0.124 | 0.104 | BCC | SS | [41] |
| TiZrHfTa | 11.53 | 1.68 | 11.54 | 1.095 | 4.08 | 0.690 | 0.104 | 0.123 | BCC | SS | [41] |
| (MoTa)6.2(NbTiZr)93.8 | 10.87 | 1.78 | 14.18 | 1.154 | 4.17 | 0.624 | 0.161 | 0.133 | BCC | SS | [42] |
| Ti50Zr25Nb15Mo10 | 10.4 | -0.56 | 39.4 | 1.154 | 4.26 | 0.552 | 0.222 | 0.137 | BCC | SS | [43] |
| Ti58Zr23Nb12Mo7 | 9.1 | -0.28 | 70.86 | 1.154 | 4.01 | 0.564 | 0.193 | 0.131 | BCC | SS | [43] |
| (MoTa)11.8(NbTiZr)88.2 | 11.75 | 1.15 | 24.24 | 1.154 | 4.25 | 0.649 | 0.191 | 0.135 | BCC | SS | [43] |
| (MoTa)16.6(NbTiZr)83.4 | 12.32 | 0.61 | 48.49 | 1.154 | 4.31 | 0.662 | 0.213 | 0.137 | BCC | SS | [43] |
| HfTiZrSn | 11.53 | -35.33 | 0.57 | 1.094 | 3.36 | 1.019 | 0.263 | 0.148 | BCC+HCP+IM | SS+IM | [44] |
| (CrCoNi)96.8Ta3.2 | 10.02 | -7.17 | 2.70 | 1.196 | 3.22 | 0.963 | 0.123 | 0.109 | FCC+laves | SS+IM | [45] |
| (CrCoNi)90.9Ta9.1 | 10.84 | -10.68 | 2.04 | 1.195 | 4.84 | 0.462 | 0.139 | 0.164 | FCC+laves | SS+IM | [45] |
| (CrCoNi)88.2Ta11.8 | 11.07 | -12.11 | 1.88 | 1.195 | 5.35 | 0.386 | 0.146 | 0.181 | FCC+laves | SS+IM | [45] |
| (CrCoNi)85.7Ta14.3 | 11.24 | -13.36 | 1.75 | 1.194 | 5.75 | 0.339 | 0.151 | 0.193 | FCC+laves | SS+IM | [45] |
| (CrCoNi)81.1Ta18.9 | 11.44 | -15.42 | 1.6 | 1.194 | 6.35 | 0.283 | 0.159 | 0.210 | FCC+laves | SS+IM | [45] |
| Ni42.6Co21.3Fe21.3V10.5Mo4.3 | 11.6 | -6.64 | 3.23 | 1.132 | 3.22 | 1.114 | 0.103 | 0.103 | FCC | SS | [46] |
| Zr44.44Hf33.33Ti5.56Nb16.67 | 9.86 | 1.97 | 11.74 | 1.094 | 3.34 | 0.880 | 0.112 | 0.096 | BCC | SS | [47] |
| Zr44.44Hf22.22Ti16.67Nb16.67 | 10.74 | 1.84 | 13.35 | 1.095 | 3.84 | 0.724 | 0.119 | 0.115 | BCC | SS | [47] |
| Fe40Cr25Ni15Al15Co5 | 11.91 | -14.09 | 1.48 | 1.158 | 4.65 | 0.548 | 0.1 | 0.145 | BCC+B2 | SS+IM | [48] |
| CoNiCu | 9.13 | 3.7 | 3.99 | 1.025 | 1.12 | 7.250 | 0.012 | 0.033 | FCC | SS | [49] |
| (FeCoNi)86.93Al6.17Ti6.9 | 11.92 | -13.61 | 1.60 | 1.195 | 5.13 | 0.452 | 0.120 | 0.167 | FCC+L21 | SS+IM | [50] |
| Mg62Li13Zn12Cu10Y3 | 9.57 | -4.52 | 1.91 | 1.458 | 7.91 | 0.152 | 0.245 | 0.210 | SS+IM | SS+IM | [51] |
| Mg43(MnAlZnCu)57 | 12.25 | -4.89 | 2.59 | 1.268 | 8.48 | 0.169 | 0.207 | 0.269 | HCP+IM+Icosahedral | SS+IM | [52] |
| Mg45.6(MnAlZnCu)54.4 | 12 | -4.51 | 2.75 | 1.268 | 8.47 | 0.166 | 0.207 | 0.267 | HCP+IM+Icosahedral | SS+IM | [52] |
| Mg50(MnAlZnCu)50 | 11.53 | -3.89 | 3.03 | 1.267 | 8.41 | 0.162 | 0.206 | 0.261 | HCP+IM+Icosahedral | SS+IM | [52] |
| Ti48.9Zr32Nb12.6Ta6.5 | 9.59 | 1.39 | 15.11 | 1.096 | 4.01 | 0.595 | 0.103 | 0.132 | BCC | SS | [53] |
| Ti31.67Zr31.67Nb31.67Ta5 | 10.33 | 2.55 | 9.41 | 1.096 | 4.00 | 0.644 | 0.112 | 0.129 | BCC | SS | [54] |
| Ti35Zr35Nb25Ta5 | 10.24 | 2.25 | 10.33 | 1.096 | 4.09 | 0.611 | 0.112 | 0.132 | BCC | SS | [54] |
| Ti45Zr45Nb5Ta5 | 8.47 | 0.72 | 24.91 | 1.095 | 4.23 | 0.472 | 0.106 | 0.136 | BCC | SS | [54] |
| Ti21.67Zr21.67Nb21.67Ta35 | 11.32 | 2.33 | 12.77 | 1.096 | 3.57 | 0.885 | 0.093 | 0.116 | BCC | SS | [54] |
| Ti15Zr15Nb35Ta35 | 10.84 | 2.1 | 14.07 | 1.096 | 3.11 | 1.116 | 0.088 | 0.102 | BCC | SS | [54] |
| Ta3.2(TiZrHf)96.8 | 10.02 | 0.18 | 125.8 | 1.095 | 3.86 | 0.670 | 0.106 | 0.117 | HCP | SS | [54] |
| Ta6.3(TiZrHf)93.7 | 10.51 | 0.44 | 54.01 | 1.095 | 3.91 | 0.684 | 0.106 | 0.119 | HCP | SS | [54] |
| Ta9.1(TiZrHf)90.9 | 10.84 | 0.67 | 37.04 | 1.095 | 3.95 | 0.691 | 0.106 | 0.120 | HCP+BCC | SS | [54] |
| Ta11.8(TiZrHf)88.2 | 11.07 | 0.87 | 29.41 | 1.095 | 3.99 | 0.694 | 0.106 | 0.120 | HCP+BCC | SS | [54] |
| Ta14.3(TiZrHf)85.7 | 11.24 | 1.05 | 25.07 | 1.095 | 4.02 | 0.695 | 0.106 | 0.121 | HCP+BCC | SS | [54] |
| Ta16.7(TiZrHf)83.3 | 11.36 | 1.21 | 22.27 | 1.095 | 4.04 | 0.695 | 0.105 | 0.122 | HCP+BCC | SS | [54] |
| Ta18.9(TiZrHf)81.1 | 11.44 | 1.35 | 20.32 | 1.095 | 4.05 | 0.694 | 0.105 | 0.122 | BCC | SS | [54] |
| Ta21.1(TiZrHf)78.9 | 11.49 | 1.47 | 18.88 | 1.095 | 4.07 | 0.693 | 0.104 | 0.122 | BCC | SS | [54] |
| TaTiZrHf | 11.53 | 1.68 | 16.91 | 1.095 | 4.08 | 0.690 | 0.104 | 0.123 | BCC | SS | [54] |
| (TiZrHf)93.7Nb6.3 | 10.51 | 0.66 | 35.58 | 1.095 | 3.91 | 0.684 | 0.115 | 0.119 | BCC+HCP | SS | [54] |
| (TiZrHf)88.2Nb11.8 | 11.07 | 1.26 | 19.84 | 1.095 | 3.99 | 0.694 | 0.120 | 0.121 | BCC | SS | [54] |
| (TiZrHf)78.9Nb21.1 | 11.49 | 2.09 | 12.68 | 1.095 | 4.07 | 0.693 | 0.127 | 0.123 | BCC | SS | [54] |
| TiZrHfNb | 11.53 | 2.38 | 11.30 | 1.095 | 4.08 | 0.690 | 0.129 | 0.123 | BCC | SS | [54] |
| (TaNb)11.8(TiZrHf)88.2 | 11.75 | -3.29 | 8.16 | 1.095 | 3.99 | 0.736 | 0.114 | 0.121 | BCC+HCP | SS | [54] |
| (CoCrNi)94.9Cu5.1 | 10.34 | -3.1 | 6.21 | 1.034 | 1.48 | 4.707 | 0.110 | 0.041 | FCC | SS | [55] |
| (CoCrNi)90.1Cu9.9 | 10.91 | -1.43 | 14.03 | 1.034 | 1.46 | 5.060 | 0.108 | 0.041 | FCC | SS | [55] |
| (CoCrNi)80Cu20 | 11.47 | 1.53 | 13.37 | 1.034 | 1.43 | 5.594 | 0.105 | 0.040 | 2 FCC | SS | [55] |
| CoCrNiCu | 11.53 | 2.74 | 7.40 | 1.034 | 1.40 | 5.809 | 0.103 | 0.039 | 2 FCC | SS | [55] |
| VCrMo | 9.13 | -0.69 | 32.18 | 1.092 | 3.33 | 0.819 | 0.243 | 0.105 | BCC | SS | [56] |
| VCrMoNb | 11.53 | -3.82 | 7.54 | 1.151 | 4.79 | 0.5 | 0.230 | 0.148 | BCC | SS | [56] |
| VCrMoTa | 11.53 | -3.52 | 8.64 | 1.151 | 4.79 | 0.5 | 0.251 | 0.149 | BCC | SS | [56] |
| CuZnMnNi | 11.53 | -8.94 | 1.70 | 1.103 | 4.06 | 0.697 | 0.156 | 0.128 | BCC+FCC | SS | [57] |
| Cu40(ZnMnNi)60 | 11.08 | -5.48 | 2.68 | 1.103 | 3.83 | 0.754 | 0.151 | 0.118 | FCC | SS | [57] |
| Mo7.5Fe55Co18Cr12.5Ni7 | 10.62 | -2.23 | 9.17 | 1.132 | 3.01 | 1.169 | 0.111 | 0.092 | FCC+µ | SS+IM | [58] |
| CrNiTi | 9.13 | -21.37 | 0.83 | 1.192 | 7.15 | 0.178 | 0.154 | 0.218 | BCC+HCP+IM | SS+IM | [59] |
| DyHoCo | 9.13 | -20 | 0.79 | 1.422 | 14.77 | 0.041 | 0.308 | 0.388 | AM | AM | [60] |
| AlCrFeTI | 10.33 | -30.27 | 0.49 | 1.179 | 5.74 | 0.313 | 0.090 | 0.156 | BCC+IM | SS+IM | [61] |
| (CoCr)80Ni20 | 8.77 | -3.55 | 4.76 | 1.034 | 1.54 | 3.660 | 0.113 | 0.042 | FCC+HCP | SS | [62] |
| (CoCr)76.9Ni23.1 | 8.92 | -3.76 | 4.54 | 1.034 | 1.53 | 3.773 | 0.113 | 0.042 | FCC+HCP | SS | [62] |
| (CoCr)74.1Ni25.9 | 9.03 | -3.94 | 4.37 | 1.034 | 1.52 | 3.870 | 0.112 | 0.042 | FCC+HCP | SS | [62] |
| (CoCr)71.4Ni28.6 | 9.09 | -4.08 | 4.24 | 1.034 | 1.51 | 3.955 | 0.112 | 0.041 | FCC | SS | [62] |
| (CoCr)69Ni31 | 9.12 | -4.19 | 4.12 | 1.034 | 1.50 | 4.031 | 0.111 | 0.041 | FCC | SS | [62] |
| Cr26Fe24Al50 | 8.64 | -21.28 | 0.59 | 1.145 | 5.76 | 0.260 | 0.089 | 0.165 | BCC+FCC | SS | [63] |
| Fe40Co30Ni30 | 9.05 | -1.56 | 10.26 | 1.008 | 0.39 | 59.317 | 0.033 | 0.033 | FCC | SS | [64] |
| Fe47.05Co32.52Ni20.43 | 8.68 | -1.35 | 11.48 | 1.008 | 0.39 | 54.87 | 0.032 | 0.033 | BCC | SS | [65] |
| Zr50Ti35Nb15 | 8.3 | 1.44 | 12.40 | 1.095 | 4.23 | 0.463 | 0.115 | 0.134 | BCC | SS | [66] |
| Fe30Co40Ni30 | 9.05 | -1.56 | 10.23 | 1.008 | 0.36 | 67.683 | 0.031 | 0.031 | FCC | SS | [67] |
| Gd55Co22.5Al22.5 | 8.31 | -38.91 | 0.31 | 1.458 | 14.60 | 0.038 | 0.285 | 0.398 | AM | AM | [68] |
| Fe40Mn40Co10Cr10 | 9.92 | -0.61 | 27.96 | 1.103 | 4.06 | 0.599 | 0.138 | 0.028 | FCC | SS | [69] |
| FeAlCrV | 11.53 | -14.6 | 1.40 | 1.146 | 4.87 | 0.485 | 0.086 | 0.142 | BCC+FCC+IM | SS+IM | [70] |
| FeAlCrMo | 11.53 | -10.18 | 2.21 | 1.145 | 5.32 | 0.406 | 0.215 | 0.152 | BCC+FCC+IM | SS+IM | [70] |
| AlFeTiV | 11.53 | -25.91 | 0.76 | 1.179 | 5.83 | 0.338 | 0.107 | 0.154 | FCC+BCC | SS | [71] |
| CuZrAl | 9.13 | -38.89 | 0.34 | 1.271 | 9.09 | 0.110 | 0.232 | 0.273 | FCC+IM | SS+IM | [72] |
| CuZrAlTi | 11.53 | -34.25 | 0.66 | 1.179 | 6.37 | 0.283 | 0.118 | 0.155 | FCC+IM | SS+IM | [72] |
| MoNbTaV | 11.53 | -3.11 | 10.29 | 1.095 | 3.56 | 0.907 | 0.257 | 0.108 | BCC | SS | [73] |
| Zr55Cu30Al10Ni5 | 8.9 | -33.62 | 0.46 | 1.299 | 10.25 | 0.084 | 0.264 | 0.291 | AM | AM | [74] |
| Cu60Zr20Hf10Ti10 | 9.05 | -16.74 | 0.91 | 1.275 | 10.32 | 0.084 | 0.264 | 0.32 | AM | AM | [75] |
| Zr58.75Cu21.15Fe4.7Al9.4Nb6 | 9.78 | -26.65 | 0.68 | 1.286 | 9.30 | 0.112 | 0.239 | 0.256 | AM | AM | [76] |
| Zr57Cu15.4Al10Ni12.6Nb5 | 10.39 | -36.78 | 0.52 | 1.297 | 9.83 | 0.107 | 0.250 | 0.274 | AM | AM | [77] |
| Zr48Cu36Al8Ag8 | 9.35 | -27.92 | 0.56 | 1.269 | 9.97 | 0.093 | 0.275 | 0.289 | AM | AM | [77] |
| Zr53Al11.6Ni11.7Cu23.7 | 9.8 | -38.95 | 0.44 | 1.299 | 10.43 | 0.09 | 0.264 | 0.297 | AM | AM | [78] |
| Pt57.5P22.5Cu14.7Ni5.3 | 9.07 | -36 | 0.38 | 1.279 | 9.04 | 0.110 | 0.117 | 0.347 | AM | AM | [79] |
| Cu57Zr23.75Ti14.25Ni5 | 9.06 | -17.71 | 0.83 | 1.308 | 10.02 | 0.09 | 0.246 | 0.318 | AM | AM | [80] |
| Zr58Co25Al15Cr2 | 8.52 | -47.32 | 0.33 | 1.298 | 10.16 | 0.082 | 0.234 | 0.279 | AM | AM | [81] |
| Zr57Co25Al15Cr3 | 8.79 | -47.02 | 0.34 | 1.298 | 10.23 | 0.083 | 0.234 | 0.282 | AM | AM | [81] |
| Zr56Co25Al15Cr4 | 9.02 | -46.71 | 0.35 | 1.298 | 10.30 | 0.084 | 0.233 | 0.285 | AM | AM | [81] |
| Ni58.8Nb14.7Zr14.7Ti9.8Co2 | 9.83 | -35.01 | 0.54 | 1.310 | 10.10 | 0.096 | 0.221 | 0.322 | AM | AM | [82] |
| Cu42.14Zr47.04Al8.82Nd2 | 8.41 | -28.36 | 0.48 | 1.462 | 10.95 | 0.07 | 0.276 | 0.325 | AM | AM | [83] |
| Cu41.71Zr46.56Al8.73Nd3 | 8.64 | -28.59 | 0.50 | 1.462 | 11.14 | 0.069 | 0.278 | 0.333 | AM | AM | [83] |
| Cu41.28Zr46.08Al8.64Nd4 | 8.83 | -28.33 | 0.52 | 1.461 | 11.32 | 0.068 | 0.280 | 0.34 | AM | AM | [83] |
| Zr60.5Ti3Al9Fe4.5Cu23 | 9.17 | -28.23 | 0.58 | 1.286 | 9.52 | 0.101 | 0.245 | 0.262 | AM | AM | [84] |
| La55Al25Cu10Ni5Co5 | 10.02 | -37.86 | 0.31 | 1.532 | 16.18 | 0.038 | 0.331 | 0.428 | AM | AM | [85] |
| Hf48Cu29Ni10Al13 | 10.03 | -32.51 | 0.51 | 1.292 | 10.22 | 0.096 | 0.279 | 0.287 | AM | AM | [86] |
| Zr57Cu20Al10Ni8Ag5 | 10.18 | -27.74 | 0.65 | 1.297 | 9.71 | 0.107 | 0.264 | 0.272 | AM | AM | [87] |
| MoRhRu | 9.13 | -12.44 | 1.89 | 1.048 | 2.07 | 2.111 | 0.049 | 0.063 | HCP | SS | [88] |
| (CoFeNi)92.3Si7.7 | 10.69 | -9.87 | 1.90 | 1.072 | 1.98 | 2.725 | 0.032 | 0.197 | FCC | SS | [89] |
| (CoFeNi)85.7Si14.3 | 11.24 | -16.24 | 1.21 | 1.072 | 2.53 | 1.74 | 0.031 | 0.246 | FCC+IM | SS+IM | [89] |
| (CoFeNi)80Si20 | 11.47 | -20.9 | 0.96 | 1.072 | 3.22 | 1.105 | 0.031 | 0.269 | FCC+IM | SS+IM | [89] |
| AlCuNi | 9.13 | -17.56 | 0.69 | 1.156 | 5.96 | 0.256 | 0.139 | 0.189 | FCC+B2 | SS+IM | [90] |
| Al31.25Li15.6Mg31.25Sn6.3Zn15.6 | 2.31 | -3.62 | 2.68 | 1.180 | 6.10 | 0.330 | 0.266 | 0.187 | FCC+IM | SS+IM | [91] |
| NbTaTiV | 11.53 | -0.08 | 387.9 | 1.095 | 3.60 | 0.885 | 0.050 | 0.104 | BCC | SS | [92] |
| NbTiVZr | 11.53 | -0.15 | 168.7 | 1.2 | 6 | 0.319 | 0.117 | 0.185 | BCC | SS | [93] |
| Nb20Ti20V40Zr20 | 11.08 | -1.11 | 22.35 | 1.202 | 6.42 | 0.268 | 0.112 | 0.201 | 3 BCC | SS | [93] |
| MoNbTaW | 11.08 | -6.55 | 5.55 | 1.053 | 2.27 | 2.228 | 0.252 | 0.069 | BCC | SS | [94] |
| VNbTi | 9.13 | -0.32 | 66.41 | 1.095 | 3.95 | 0.583 | 0.037 | 0.115 | BCC | SS | [95] |
| Cr12Ni12Mn12Fe64 | 8.72 | -1.56 | 10.14 | 1.316 | 8.45 | 1.355 | 0.108 | 0.028 | FCC | SS | [96] |
| Cr12Ni12Mn16Fe60 | 9.22 | -1.59 | 10.41 | 1.314 | 9.42 | 1.43 | 0.117 | 0.029 | FCC | SS | [96] |
| Cr12Ni12Mn20Fe66 | 9.61 | -1.63 | 10.52 | 1.313 | 10.16 | 1.49 | 0.124 | 0.03 | FCC | SS | [96] |
| Nb31Ti34Zr26Al6V3 | 11.26 | -7.33 | 3.35 | 1.199 | 4.3 | 0.6 | 0.11 | 0.137 | BCC | SS | [97] |
| Nb31Ti32Zr26Al6V5 | 11.61 | -7.45 | 3.41 | 1.199 | 4.51 | 0.56 | 0.112 | 0.142 | BCC | SS | [97] |
| Nb31Ti30Zr26Al6V7 | 11.88 | -7.57 | 3.45 | 1.199 | 4.72 | 0.53 | 0.113 | 0.148 | BCC | SS | [97] |
| Nb31Ti28Zr26Al6V9 | 12.1 | -7.68 | 3.47 | 1.199 | 4.91 | 0.5 | 0.114 | 0.153 | BCC | SS | [97] |
| Nb31Ti26Zr26Al6V11 | 12.26 | -7.78 | 3.48 | 1.199 | 5.09 | 0.47 | 0.115 | 0.158 | BCC | SS | [97] |
| MoReRu | 9.13 | -9.79 | 2.78 | 1.048 | 1.78 | 2.857 | 0.133 | 0.056 | HCP | SS | [98] |
| Ti10Fe30Co30Ni30 | 10.92 | -10.26 | 1.90 | 1.196 | 5.11 | 1.697 | 0.104 | 0.163 | FCC+B2+L12 | SS+IM | [99] |
| (NiCoCr)92Al6Ta2 | 11.09 | -11.88 | 1.51 | 1.195 | 4.02 | 0.683 | 0.125 | 0.135 | FCC+IM | SS+IM | [100] |
| (CoCrNi)91Al9 | 10.83 | -13.1 | 1.49 | 1.159 | 4 | 0.679 | 0.121 | 0.133 | FCC+IM | SS+IM | [101] |
| (VCoNi)91Al9 | 10.84 | -21.49 | 0.91 | 1.158 | 4.75 | 0.48 | 0.132 | 0.148 | FCC+BCC | SS | [102] |
| (VCr)33.4(CoNi)66.6 | 11.05 | -9.82 | 2.13 | 1.087 | 2.92 | 1.29 | 0.118 | 0.089 | FCC+HCP | SS | [103] |
| (CoCrNi)96.8Ta3.2 | 10.02 | -7.17 | 2.7 | 1.196 | 3.22 | 0.96 | 0.123 | 0.109 | FCC+laves | SS+IM | [104] |
| CoNiV | 9.13 | -14.19 | 1.21 | 1.158 | 3.67 | 0.676 | 0.125 | 0.110 | FCC | SS | [105] |
| (CoNiV)97Al3 | 9.98 | -16.79 | 1.10 | 1.158 | 4.09 | 0.549 | 0.128 | 0.126 | FCC | SS | [105] |
| (CoNiV)95Al5 | 10.33 | -18.42 | 1.03 | 1.158 | 4.33 | 0.549 | 0.129 | 0.134 | FCC+B2 | SS+IM | [105] |
| (CoFe)70.6Al17.6Cr11.8 | 10.75 | -15.56 | 1.16 | 1.158 | 5.10 | 0.412 | 0.105 | 0.159 | BCC+ L21 | SS+IM | [106] |
| Fe50Mn25Cr15Ni10 | 10.04 | -1.49 | 12.05 | 1.104 | 3.64 | 0.757 | 0.13 | 0.029 | FCC | SS | [107] |
| Fe50Mn25Cr15(NiCo)10 | 10.62 | -1.18 | 16.13 | 1.104 | 3.64 | 0.801 | 0.128 | 0.027 | FCC+HCP | SS | [107] |
| Fe50Mn25Cr15Co10 | 10.04 | -0.86 | 20.88 | 1.104 | 3.64 | 0.757 | 0.126 | 0.026 | FCC+HCP | SS | [107] |
| VNbTiSi | 11.53 | -38.83 | 0.63 | 1.262 | 8.68 | 0.152 | 0.138 | 0.128 | BCC+IM | SS+IM | [108] |
| (CoCrNi)94Al3Ti3 | 10.82 | -10.28 | 1.96 | 1.196 | 3.78 | 0.756 | 0.122 | 0.124 | FCC+ L12 | SS+IM | [109] |
| (NiY)66.6Al30.4Ti3 | 9.97 | -47.33 | 0.31 | 1.5 | 15.82 | 0.039 | 0.282 | 0.462 | AM | AM | [110] |
| (NiY)66.6Al27.4Ti6 | 10.44 | -46.14 | 0.35 | 1.499 | 15.79 | 0.041 | 0.282 | 0.460 | AM | AM | [110] |
| (NiY)66.6Al24.4Ti9 | 10.75 | -44.66 | 0.37 | 1.499 | 15.76 | 0.043 | 0.282 | 0.459 | AM | AM | [110] |
| (NiY)66.6Al21.4Ti12 | 10.95 | -42.9 | 0.41 | 1.499 | 15.73 | 0.044 | 0.282 | 0.458 | AM | AM | [110] |
| (NiY)66.6Al18.4Ti15 | 11.05 | -40.84 | 0.44 | 1.499 | 15.70 | 0.044 | 0.282 | 0.457 | AM | AM | [110] |
| (NiY)66.6Al15.4Ti18 | 11.05 | -38.49 | 0.47 | 1.499 | 15.67 | 0.045 | 0.282 | 0.455 | AM | AM | [110] |
| (NiY)66.6Al12.4Ti21 | 10.97 | -35.84 | 0.51 | 1.498 | 15.63 | 0.044 | 0.282 | 0.454 | AM | AM | [110] |
| V47Fe11Ti30Cr10La2 | 10.54 | -4.42 | 4.88 | 1.568 | 7.33 | 0.196 | 0.111 | 0.254 | BCC+laves | SS+IM | [111] |
| V47Fe11Ti30Cr10Ce2 | 10.54 | -4.59 | 4.70 | 1.518 | 6.98 | 0.215 | 0.109 | 0.234 | BCC+laves | SS+IM | [111] |
| V47Fe11Ti30Cr10Y2 | 10.54 | -4.82 | 4.5 | 1.508 | 6.92 | 0.219 | 0.1 | 0.225 | BCC+laves | SS+IM | [111] |
| V47Fe11Ti30Cr10Sc2 | 10.54 | -5.53 | 3.92 | 1.335 | 5.89 | 0.303 | 0.091 | 0.175 | BCC+laves | SS+IM | [111] |
| CoNiFe | 9.13 | -1.03 | 15.67 | 1.008 | 0.38 | 2 | 0.033 | 0.032 | FCC | SS | [112] |
| Fe42.8Cr28.6(NiCu)28.6 | 10.62 | 3.29 | 5.93 | 1.034 | 1.19 | 2 | 0.095 | 0.028 | FCC+BCC | SS | [113] |
| Fe42.1Cr28.1(NiCu)28Al1.8 | 11.17 | 1.71 | 11.87 | 1.159 | 2.02 | 2 | 0.098 | 0.061 | FCC+BCC | SS | [113] |
| Fe41.4Cr27.6(NiCu)27.6Al3.4 | 11.5 | 0.25 | 84.85 | 1.159 | 2.56 | 1.742 | 0.1 | 0.079 | FCC+BCC | SS | [113] |
| Fe40Cr26.7(NiCu)26.6Al6.7 | 11.95 | -2.41 | 8.82 | 1.158 | 3.31 | 1.084 | 0.104 | 0.104 | FCC+BCC | SS | [113] |
| (FeNi)60(AlCr)40 | 11.36 | -18.75 | 1.02 | 1.158 | 5.24 | 0.413 | 0.12 | 0.165 | BCC+B2 | SS+IM | [114] |
| Co35Cr30Ni27Al4Ti4 | 11.14 | -11.76 | 1.75 | 1.195 | 4.23 | 0.621 | 0.124 | 0.139 | FCC+ L12 | SS+IM | [115] |
| ScGdHo | 9.13 | 0.71 | 22.14 | 1.098 | 3.61 | 0.697 | 0.069 | 0.116 | HCP | SS | [116] |
| (TiNb)75Zr25 | 9 | 2.51 | 8.22 | 1.096 | 3.74 | 0.64 | 0.107 | 0.123 | BCC | SS | [117] |
| (TiZr)75Nb25 | 9 | 2.1 | 9.50 | 1.095 | 4.14 | 0.523 | 0.115 | 0.134 | BCC | SS | [117] |
| Fe20Cr20Ni30Al30 | 11.36 | -23.97 | 0.75 | 1.1571 | 5.87 | 0.328 | 0.128 | 0.182 | BCC+B2 | SS+IM | [118] |
| (TiZr)90Nb7Sn3 | 8.4 | -4.52 | 3.79 | 1.095 | 4.20 | 0.474 | 0.139 | 0.144 | BCC | SS | [119] |
| (TiZr)90Nb5Sn5 | 8.47 | -8.06 | 2.09 | 1.095 | 4.18 | 0.484 | 0.154 | 0.149 | BCC | SS | [119] |
| (TiZr)90Nb3Sn7 | 8.4 | -11.56 | 1.41 | 1.095 | 4.15 | 0.486 | 0.168 | 0.152 | BCC | SS | [119] |
| (NbTiZr)96.8(MoTa)3.2 | 10.21 | 2.14 | 10.97 | 1.154 | 4.11 | 0.602 | 0.141 | 0.132 | BCC | SS | [120] |
| (CrCoNi)83.3Mo16.7 | 11.36 | -5.67 | 4.12 | 1.131 | 4.18 | 0.649 | 0.163 | 0.135 | FCC+laves+ σ | SS+IM | [121] |
| (CrTaTi)89.6Al10.4 | 10.96 | -15.92 | 1.59 | 1.149 | 5.7 | 0.337 | 0.065 | 0.163 | BCC+IM | SS+IM | [122] |
| MoNbV | 9.13 | -2.94 | 8.11 | 1.096 | 3.49 | 0.746 | 0.257 | 0.108 | BCC | SS | [123] |
| MoNbVTi | 11.53 | -2.45 | 11.50 | 1.095 | 3.56 | 0.907 | 0.248 | 0.103 | BCC | SS | [123] |
| Fe65Cr15(CoNi)12Si8 | 9.18 | -10.09 | 1.68 | 1.099 | 2.027 | 2 | 0.071 | 0.183 | BCC+FCC | SS | [124] |
| (CrFeNi)88.2Nb11.8 | 11.07 | -10.55 | 2.1 | 1.195 | 5.224 | 0.405 | 0.117 | 0.171 | FCC+laves | SS+IM | [125] |
| (CrFeNi)78.1Nb21.1 | 11.49 | -14.22 | 1.68 | 1.193 | 6.434 | 0.277 | 0.123 | 0.204 | FCC+laves | SS+IM | [125] |
| (CrFeNi)85.7Nb14.3 | 11.24 | -11.66 | 1.95 | 1.194 | 5.624 | 0.355 | 0.119 | 0.182 | FCC+laves | SS+IM | [125] |
| (CrFeNi)83.3Nb16.7 | 11.36 | -12.63 | 1.84 | 1.194 | 5.947 | 0.321 | 0.120 | 0.191 | FCC+laves | SS+IM | [125] |
| (CrFeNi)81.1Nb18.9 | 11.44 | -13.48 | 1.75 | 1.194 | 6.213 | 0.296 | 0.122 | 0.198 | FCC+laves | SS+IM | [125] |
| (CoNi)74V16Mo10 | 10.47 | -9.43 | 2.14 | 1.131 | 4.195 | 0.594 | 0.134 | 0.133 | FCC+ µ | SS+IM | [126] |

**Table S2:** Dataset used for binary classifications B1 (SS, SS+IM) and B2 (SSS, MSS)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Medium entropy alloy composition** | **(KJ/mol)** |  |  |  | **VEC** | **Phase name** | **Phase category** | **Reference** |
| FeCrNiAl | -21.02 | 1.56 | 5.52 | 0.377 | 5.57 | BCC+B2 | SS+IM | [1] |
| Fe35(CrNiAl)65 | -11.5 | 1.65 | 5.31 | 0.4 | 6.916 | BCC+B2 | SS+IM | [1] |
| Fe45(CrNiAl)55 | -9.81 | 1.86 | 5.04 | 0.422 | 7.083 | BCC+B2 | SS+IM | [1] |
| Fe55(CrNiAl)45 | -8.09 | 2.09 | 4.70 | 0.444 | 7.25 | BCC+B2 | SS+IM | [1] |
| Fe65(CrNiAl)35 | -6.35 | 2.35 | 4.26 | 0.47 | 7.416 | BCC+B2 | SS+IM | [1] |
| CrCoNi | -4.28 | 4.03 | 1.49 | 4.099 | 8.33 | FCC | SSS | [2] |
| FeCrNiCo | -3.71 | 5.80 | 1.29 | 6.835 | 8.25 | FCC | SSS | [3] |
| FeCrNiMn | -3.83 | 5.44 | 3.64 | 0.867 | 7.75 | FCC+BCC | MSS | [3] |
| FeNiCoMn | -3.82 | 5.14 | 3.95 | 0.738 | 8.5 | FCC | SSS | [3] |
| FeCoCrMn | -2.29 | 9.16 | 3.64 | 0.867 | 7.5 | FCC+BCC | MSS | [3] |
| NiCoCrMn | -5.6 | 3.69 | 3.79 | 0.799 | 8 | FCC | SSS | [3] |
| FeNiCo | -1.62 | 9.97 | 0.37 | 64.565 | 9 | FCC | SSS | [3] |
| FeNiCr | -4.28 | 4.06 | 1.34 | 5.072 | 8 | FCC | SSS | [3] |
| FeNiMn | -4.17 | 3.69 | 4.20 | 0.516 | 8.33 | FCC | SSS | [3] |
| FeCoMn | -2.4 | 6.46 | 4.20 | 0.516 | 8 | FCC+BCC | MSS | [3] |
| NiCoMn | -5.99 | 2.55 | 4.38 | 0.474 | 8.67 | FCC | SSS | [3] |
| NiCrMn | -5.61 | 2.94 | 3.82 | 0.623 | 7.67 | FCC | SSS | [3] |
| CoCrMn | -3.3 | 5.03 | 3.82 | 0.623 | 7.33 | FCC++IM | SS+IM | [3] |
| WNbMoTa | -6.55 | 5.55 | 2.27 | 2.228 | 5.5 | BCC | SSS | [4] |
| CuFeMn | 7.49 | 1.90 | 3.67 | 0.677 | 8.67 | Dual FCC | MSS | [6] |
| Al7.5(CuFeMn)92.5 | 0.75 | 21.63 | 4.33 | 0.568 | 8.2416 | BCC+FCC | MSS | [6] |
| Al15(CuFeMn)85 | -4.99 | 3.31 | 4.77 | 0.494 | 7.8166 | BCC+FCC | MSS | [6] |
| Fe57.5(CoNi)32.5Cr10 | -1.86 | 9.28 | 0.87 | 12.274 | 8.2875 | FCC | SSS | [7] |
| Fe60(CoNi)30Cr10 | -1.79 | 9.39 | 0.86 | 12.164 | 8.25 | FCC | SSS | [7] |
| Fe62.5(CoNi)27.5Cr10 | -1.71 | 9.51 | 0.85 | 12.026 | 8.2125 | FCC+BCC | MSS | [7] |
| Fe60(MnCoNiCr)40 | -1.68 | 10.97 | 2.69 | 1.404 | 8 | FCC | SSS | [7] |
| Fe65(MnCoNiCr)35 | -1.43 | 11.91 | 2.54 | 1.454 | 8 | FCC+HCP | MSS | [7] |
| Fe70(MnCoNiCr)30 | -1.19 | 12.97 | 2.37 | 1.512 | 8 | FCC+BCC+HCP | MSS | [7] |
| (CrFeNi)93.75Al6.25 | -9.58 | 2.02 | 3.35 | 0.934 | 7.6875 | FCC | SSS | [8] |
| (CrFeNi)88.2Al11.8 | -13.64 | 1.45 | 4.27 | 0.605 | 7.411 | FCC+BCC+B2 | SS+IM | [8] |
| (CrFeNi)83.4Al8.3Ti8.3 | -16.36 | 1.37 | 5.43 | 0.416 | 7.25 | FCC+BCC+B2 | SS+IM | [8] |
| (CrFeNi)83.4Al11.1Ti5.5 | -16.75 | 1.31 | 5.25 | 0.443 | 7.222 | FCC+BCC+B2 | SS+IM | [8] |
| Co17.5Cr12.5Fe55Ni10Mo5 | -2.21 | 9.06 | 2.56 | 1.612 | 8.025 | FCC | SSS | [9] |
| Co18Cr12.5Fe55Ni7Mo7.5 | -2.23 | 3.17 | 3.01 | 1.169 | 7.92 | FCC | SSS | [9] |
| TiZrHf | -0.12 | 164.9 | 3.80 | 0.631 | 4 | HCP | SSS | [10] |
| Ti40Zr20Hf10Nb20Ta10 | 2.07 | 13.79 | 3.85 | 0.823 | 4.5 | BCC | SSS | [10] |
| (CrCoNi)96.78Si3.22 | -8.76 | 2.15 | 1.87 | 2.840 | 8.1935 | FCC | SSS | [11] |
| (CrCoNi)93.75Si6.25 | -12.03 | 1.64 | 2.16 | 2.246 | 8.0625 | FCC | SSS | [11] |
| (CrCoNi)90.9Si9.1 | -14.89 | 1.36 | 2.38 | 1.904 | 7.9394 | FCC | SSS | [11] |
| Ti45(AlCrNb)55 | -22.84 | 0.91 | 4.74 | 0.476 | 4.367 | BCC+IM | SS+IM | [12] |
| Ti50(AlCrNb)50 | -21.65 | 0.92 | 4.58 | 0.490 | 4.333 | BCC+IM | SS+IM | [12] |
| Ti55(AlCrNb)45 | -20.29 | 0.94 | 4.40 | 0.506 | 4.3 | BCC+IM | SS+IM | [12] |
| Ti60(AlCrNb)40 | -18.75 | 0.96 | 4.20 | 0.522 | 4.267 | BCC | SSS | [12] |
| Ti65(AlCrNb)35 | -17.03 | 0.98 | 3.98 | 0.541 | 4.233 | BCC | SSS | [12] |
| Ti27V33Ta40 | -0.52 | 44.44 | 3.94 | 0.580 | 4.73 | BCC | SSS | [13] |
| Ti33V33Ta34 | -0.55 | 41.34 | 3.94 | 0.586 | 4.67 | BCC | SSS | [13] |
| Ti40V33Ta27 | -0.63 | 34.15 | 3.94 | 0.580 | 4.6 | BCC | SSS | [13] |
| Ti45V20Ta35 | 0 | 14119 | 3.31 | 0.791 | 4.55 | BCC | SSS | [13] |
| Ni57.6Cr19.2Fe19.2Nb4 | -7.25 | 2.31 | 3.45 | 0.751 | 8.648 | FCC | SSS | [14] |
| TiZrNbTa | 2.46 | 11.82 | 3.74 | 0.821 | 4.5 | BCC | SSS | [15] |
| Al7.5(CoCrNi)92.5 | -11.88 | 1.63 | 3.72 | 0.769 | 7.9333 | FCC | SSS | [16] |
| (CoCrNi)96.8Mo3.2 | -5.2 | 3.71 | 2.40 | 1.737 | 8.258 | FCC | SSS | [17] |
| (CoCrNi)93.75Mo6.25 | -5.34 | 3.84 | 2.97 | 1.190 | 8.1875 | FCC | SSS | [17] |
| Fe50(CoCrMnNi)50 | -2.22 | 9.38 | 2.96 | 1.314 | 8 | FCC | SSS | [18] |
| (CoCrNi)99W1 | -4.97 | 3.65 | 1.87 | 2.692 | 8.31 | FCC | SSS | [19] |
| (CoCrNi)98W2 | -4.92 | 3.82 | 2.19 | 2.033 | 8.2867 | FCC | SSS | [19] |
| (CoCrNi)97W3 | -4.87 | 3.99 | 2.45 | 1.652 | 8.2633 | FCC | SSS | [19] |
| (CoFeNi)96.8Al3.2 | -4.43 | 3.94 | 2.50 | 1.595 | 8.8064 | FCC | SSS | [20] |
| (CoFeNi)88.2Al11.8 | -12.32 | 1.50 | 4.48 | 0.551 | 8.2941 | FCC+B2/BCC | SS+IM | [20] |
| (CoFeNi)83.3Al16.7 | -16.62 | 1.14 | 5.14 | 0.429 | 8 | FCC+B2/BCC | SS+IM | [20] |
| (CoFeNi)88.2Ti11.8 | -11.68 | 1.69 | 5.46 | 0.37 | 8.4117 | FCC+BCC | MSS | [20] |
| Ni47.5Cr23.75Co23.75Ti5 | -9.01 | 2.03 | 3.83 | 0.668 | 8.5125 | FCC | SSS | [21] |
| Fe50Mn25Ni10Cr15 | -1.49 | 12.05 | 3.64 | 0.757 | 7.65 | FCC | SSS | [22] |
| Fe48.5Mn24.25Ni9.7Cr14.55Al3 | -4.24 | 4.51 | 4.01 | 0.673 | 7.5105 | FCC | SSS | [22] |
| Fe47.5Mn23.75Ni9.5Cr14.25Al5 | -5.98 | 3.26 | 4.23 | 0.625 | 7.4175 | FCC+BCC | MSS | [22] |
| Fe47Mn23.5Ni9.4Cr14.1Al6 | -6.81 | 2.88 | 4.33 | 0.604 | 7.371 | FCC+BCC | MSS | [22] |
| Fe46.5Mn23.25Ni9.3Cr13.95Al7 | -7.64 | 2.58 | 4.42 | 0.584 | 7.3245 | FCC+BCC | MSS | [22] |
| Fe46Mn23Ni9.2Cr13.8Al8 | -8.44 | 2.35 | 4.51 | 0.567 | 7.278 | FCC+BCC | MSS | [22] |
| (AlCr)33.4 Fe33.3Ni33.3 | -16.78 | 1.11 | 4.96 | 0.448 | 7.5 | FCC+BCC+B2 | SS+IM | [23] |
| Ni46Cr23Fe23Al4Ti4 | -11.36 | 1.72 | 4.19 | 0.610 | 8.1 | FCC+L12 | SS+IM | [24] |
| Ni50Cr25Co25 | -4.46 | 1.37 | 1.37 | 4.574 | 9.75 | FCC | SSS | [24] |
| Fe40Co40Ni10Al10 | -10.04 | 1.67 | 4.15 | 0.574 | 8.1 | BCC+FCC | MSS | [25] |
| Fe40Co40Ni10Mn10 | -1.74 | 10.01 | 2.76 | 1.299 | 8.5 | BCC+FCC | MSS | [25] |
| Co38Cr33Ni29 | -3.95 | 4.35 | 1.48 | 4.097 | 8.3 | FCC | SSS | [26] |
| Co42Cr33Ni25 | -3.64 | 4.65 | 1.48 | 4.038 | 8.26 | FCC | SSS | [26] |
| Hf20Nb10Ti35Zr35 | 1.01 | 23.2 | 4.09 | 0.639 | 4.2 | BCC | SSS | [27] |
| Fe7.7(CrNiAl)92.3 | -15.96 | 1.09 | 5.76 | 0.321 | 6.4615 | BCC+B2 | SS+IM | [28] |
| VCoNi | -14.79 | 1.16 | 3.67 | 0.676 | 8 | FCC | SSS | [29] |
| Ti60Mo10V10Cr10Zr10 | -3.97 | 5.40 | 5.48 | 0.339 | 4.5 | BCC | SSS | [30] |
| (CoCrNi)98.95Ce1.05 | -5.36 | 3.34 | 4.78 | 0.415 | 8.2878 | FCC | SSS | [31] |
| (CoCrNi)97.39Ce2.61 | -5.84 | 3.17 | 7.21 | 0.19 | 8.22 | FCC+HCP | MSS | [31] |
| (CoCrNi)96.8Zr3.2 | -8.82 | 2.15 | 4.88 | 0.419 | 8.1933 | FCC | SSS | [32] |
| (CoCrNi)93.7Zr6.3 | -12.15 | 1.64 | 6.50 | 0.248 | 8.062 | FCC+HCP | MSS | [32] |
| (CoCrNi)90.9Zr9.1 | -15.06 | 1.37 | 7.60 | 0.187 | 7.9394 | FCC+HCP | MSS | [32] |
| Ti44V44Cr9Al3 | -6.53 | 2.71 | 4.72 | 0.389 | 4.59 | BCC | SSS | [33] |
| Ti44V44Cr6Al6 | -9.67 | 1.82 | 4.51 | 0.432 | 4.5 | BCC | SSS | [33] |
| Ti44V44Cr3Al9 | -12.67 | 1.34 | 4.28 | 0.473 | 4.41 | BCC | SSS | [33] |
| Al9.1(CrFeNi)90.9 | -11.47 | 1.67 | 3.87 | 0.721 | 7.5454 | FCC+BCC | MSS | [34] |
| Al10.4(CrFeNi)89.6 | -12.72 | 1.55 | 4.08 | 0.655 | 7.4776 | FCC+BCC | MSS | [34] |
| Al11(CrFeNi)89 | -13.09 | 1.51 | 4.16 | 0.634 | 7.451 | FCC+BCC+B2 | SS+IM | [34] |
| Al14.3(CrFeNi)85.7 | -15.3 | 1.29 | 4.59 | 0.532 | 7.2857 | BCC+B2 | SS+IM | [34] |
| AgCuAl | -6.34 | 1.69 | 5.29 | 0.326 | 8.333 | FCC | SSS | [35] |
| Ti35Zr15Ta25Nb25 | 2.14 | 13.11 | 3.11 | 1.151 | 4.5 | BCC | SSS | [36] |
| Al50(TiCrMnV)50 | -30.33 | 0.54 | 3.91 | 0.753 | 4.25 | BCC+FCC | MSS | [37] |
| Al50Ti20Cr20Mn10 | -31.81 | 0.46 | 4.46 | 0.509 | 4.2 | FCC+BCC+IM | SS+IM | [37] |
| Al50Ti20Cr15Mn15 | -32.71 | 0.44 | 4.08 | 0.615 | 4.25 | FCC+BCC+IM | SS+IM | [37] |
| Al50Ti20Cr10Mn20 | -33.64 | 0.41 | 3.66 | 0.756 | 4.3 | FCC+BCC+IM | SS+IM | [37] |
| Al50Ti25Cr15Mn10 | -33.96 | 0.42 | 4.13 | 0.587 | 4.1 | FCC+BCC+IM | SS+IM | [37] |
| Al50Ti15Cr15Mn20 | -31.29 | 0.45 | 4.01 | 0.638 | 4.4 | FCC+BCC+IM | SS+IM | [37] |
| Al50Ti15Cr15Mn15V5 | -31.02 | 0.51 | 4.06 | 0.677 | 4.3 | FCC+BCC+IM | SS+IM | [37] |
| Al50(TiCrMn)37.5V12.5 | -30.33 | 0.54 | 3.91 | 0.753 | 4.25 | FCC+BCC+IM | SS+IM | [37] |
| Al50(TiCrMn)30V20 | -29.65 | 0.55 | 3.74 | 0.807 | 4.2 | FCC+BCC+IM | SS+IM | [37] |
| Ti60Al6(VCrNb)34 | -10.36 | 1.97 | 4.45 | 0.509 | 4.39 | BCC | SSS | [38] |
| Ti60Al8(VCrNb)32 | -12.66 | 1.60 | 4.34 | 0.540 | 4.3466 | BCC | SSS | [38] |
| Ti60Al10(VCrNb)30 | -14.89 | 1.34 | 4.22 | 0.571 | 4.3 | BCC | SSS | [38] |
| Ti60Al12(VCrNb)28 | -17.04 | 1.15 | 4.10 | 0.603 | 4.2533 | BCC+B2 | SS+IM | [38] |
| Ti60Al18(VCrNb)22 | -23.01 | 0.79 | 3.71 | 0.716 | 4.1133 | BCC+B2 | SS+IM | [38] |
| TiZrNb | 2.53 | 8.19 | 4.09 | 0.556 | 4.333 | BCC | SSS | [39] |
| Fe61Mn18Si11Cr10 | -12.33 | 1.30 | 4.13 | 0.526 | 7.18 | BCC+FCC | MSS | [40] |
| HfNbTa | 3.00 | 8.67 | 3.74 | 0.650 | 4.67 | BCC | SSS | [41] |
| TiZrHfTa | 1.68 | 11.54 | 4.08 | 0.690 | 4.25 | BCC | SSS | [41] |
| (MoTa)6.2(NbTiZr)93.8 | 1.78 | 14.18 | 4.17 | 0.624 | 4.4063 | BCC | SSS | [42] |
| Ti50Zr25Nb15Mo10 | -0.56 | 39.4 | 4.26 | 0.552 | 4.5 | BCC | SSS | [43] |
| Ti58Zr23Nb12Mo7 | -0.28 | 70.86 | 4.01 | 0.564 | 4.38 | BCC | SSS | [43] |
| (MoTa)11.8(NbTiZr)88.2 | 1.15 | 24.24 | 4.25 | 0.649 | 4.4705 | BCC | SSS | [43] |
| (MoTa)16.6(NbTiZr)83.4 | 0.61 | 48.49 | 4.31 | 0.662 | 4.5278 | BCC | SSS | [43] |
| HfTiZrSn | -35.33 | 0.57 | 3.36 | 1.019 | 4 | BCC+HCP+IM | SS+IM | [44] |
| (CrCoNi)96.8Ta3.2 | -7.17 | 2.70 | 3.22 | 0.963 | 8.2258 | FCC+laves | SS+IM | [45] |
| (CrCoNi)90.9Ta9.1 | -10.68 | 2.04 | 4.84 | 0.462 | 8.0303 | FCC+laves | SS+IM | [45] |
| (CrCoNi)88.2Ta11.8 | -12.11 | 1.88 | 5.35 | 0.386 | 7.9411 | FCC+laves | SS+IM | [45] |
| (CrCoNi)85.7Ta14.3 | -13.36 | 1.75 | 5.75 | 0.339 | 7.8571 | FCC+laves | SS+IM | [45] |
| (CrCoNi)81.1Ta18.9 | -15.42 | 1.6 | 6.35 | 0.283 | 7.7027 | FCC+laves | SS+IM | [45] |
| Ni42.6Co21.3Fe21.3V10.5Mo4.3 | -6.64 | 3.23 | 3.22 | 1.114 | 8.659 | FCC | SSS | [46] |
| Zr44.44Hf33.33Ti5.56Nb16.67 | 1.97 | 11.74 | 3.34 | 0.880 | 4.334 | BCC | SSS | [47] |
| Zr44.44Hf22.22Ti16.67Nb16.67 | 1.84 | 13.35 | 3.84 | 0.724 | 4.334 | BCC | SSS | [47] |
| Fe40Cr25Ni15Al15Co5 | -14.09 | 1.48 | 4.65 | 0.548 | 7.1 | BCC+B2 | SS+IM | [48] |
| CoNiCu | 3.7 | 3.99 | 1.12 | 7.250 | 10 | FCC | SSS | [49] |
| (FeCoNi)86.93Al6.17Ti6.9 | -13.61 | 1.60 | 5.13 | 0.452 | 7.7053 | FCC+L21 | SS+IM | [50] |
| Mg62Li13Zn12Cu10Y3 | -4.52 | 1.91 | 7.91 | 0.152 | 4 | SS+IM | SS+IM | [51] |
| Mg43(MnAlZnCu)57 | -4.89 | 2.59 | 8.48 | 0.169 | 5.5625 | HCP+IM+Icosahedral | SS+IM | [52] |
| Mg45.6(MnAlZnCu)54.4 | -4.51 | 2.75 | 8.47 | 0.166 | 5.4 | HCP+IM+Icosahedral | SS+IM | [52] |
| Mg50(MnAlZnCu)50 | -3.89 | 3.03 | 8.41 | 0.162 | 5.125 | HCP+IM+Icosahedral | SS+IM | [52] |
| Ti48.9Zr32Nb12.6Ta6.5 | 1.39 | 15.11 | 4.01 | 0.595 | 4.191 | BCC | SSS | [53] |
| Ti31.67Zr31.67Nb31.67Ta5 | 2.55 | 9.41 | 4.00 | 0.644 | 4.3671 | BCC | SSS | [54] |
| Ti35Zr35Nb25Ta5 | 2.25 | 10.33 | 4.09 | 0.611 | 4.3 | BCC | SSS | [54] |
| Ti45Zr45Nb5Ta5 | 0.72 | 24.91 | 4.23 | 0.472 | 4.1 | BCC | SSS | [54] |
| Ti21.67Zr21.67Nb21.67Ta35 | 2.33 | 12.77 | 3.57 | 0.885 | 4.5671 | BCC | SSS | [54] |
| Ti15Zr15Nb35Ta35 | 2.1 | 14.07 | 3.11 | 1.116 | 4.7 | BCC | SSS | [54] |
| Ta3.2(TiZrHf)96.8 | 0.18 | 125.8 | 3.86 | 0.670 | 4.0322 | HCP | SSS | [54] |
| Ta6.3(TiZrHf)93.7 | 0.44 | 54.01 | 3.91 | 0.684 | 4.0625 | HCP | SSS | [54] |
| Ta9.1(TiZrHf)90.9 | 0.67 | 37.04 | 3.95 | 0.691 | 4.0909 | HCP+BCC | MSS | [54] |
| Ta11.8(TiZrHf)88.2 | 0.87 | 29.41 | 3.99 | 0.694 | 4.1176 | HCP+BCC | MSS | [54] |
| Ta14.3(TiZrHf)85.7 | 1.05 | 25.07 | 4.02 | 0.695 | 4.1428 | HCP+BCC | MSS | [54] |
| Ta16.7(TiZrHf)83.3 | 1.21 | 22.27 | 4.04 | 0.695 | 4.1667 | HCP+BCC | MSS | [54] |
| Ta18.9(TiZrHf)81.1 | 1.35 | 20.32 | 4.05 | 0.694 | 4.1891 | BCC | SSS | [54] |
| Ta21.1(TiZrHf)78.9 | 1.47 | 18.88 | 4.07 | 0.693 | 4.2105 | BCC | SSS | [54] |
| TaTiZrHf | 1.68 | 16.91 | 4.08 | 0.690 | 4.25 | BCC | SSS | [54] |
| (TiZrHf)93.7Nb6.3 | 0.66 | 35.58 | 3.91 | 0.684 | 4.125 | BCC+HCP | MSS | [54] |
| (TiZrHf)88.2Nb11.8 | 1.26 | 19.84 | 3.99 | 0.694 | 4.2353 | BCC | SSS | [54] |
| (TiZrHf)78.9Nb21.1 | 2.09 | 12.68 | 4.07 | 0.693 | 4.4211 | BCC | SSS | [54] |
| TiZrHfNb | 2.38 | 11.30 | 4.08 | 0.690 | 4.5 | BCC | SSS | [54] |
| (TaNb)11.8(TiZrHf)88.2 | -3.29 | 8.16 | 3.99 | 0.736 | 4.1176 | BCC+HCP | MSS | [54] |
| (CoCrNi)94.9Cu5.1 | -3.1 | 6.21 | 1.48 | 4.707 | 8.4684 | FCC | SSS | [55] |
| (CoCrNi)90.1Cu9.9 | -1.43 | 14.03 | 1.46 | 5.060 | 8.5976 | FCC | SSS | [55] |
| (CoCrNi)80Cu20 | 1.53 | 13.37 | 1.43 | 5.594 | 8.8667 | Dual FCC | MSS | [55] |
| CoCrNiCu | 2.74 | 7.40 | 1.40 | 5.809 | 9 | Dual FCC | MSS | [55] |
| VCrMo | -0.69 | 32.18 | 3.33 | 0.819 | 5.6667 | BCC | SSS | [56] |
| VCrMoNb | -3.82 | 7.54 | 4.79 | 0.5 | 5.5 | BCC | SSS | [56] |
| VCrMoTa | -3.52 | 8.64 | 4.79 | 0.5 | 5.5 | BCC | SSS | [56] |
| CuZnMnNi | -8.94 | 1.70 | 4.06 | 0.697 | 10 | BCC+FCC | MSS | [57] |
| Cu40(ZnMnNi)60 | -5.48 | 2.68 | 3.83 | 0.754 | 10.2 | FCC | SSS | [57] |
| Mo7.5Fe55Co18Cr12.5Ni7 | -2.23 | 9.17 | 3.01 | 1.169 | 7.92 | FCC+µ | SS+IM | [58] |
| CrNiTi | -21.37 | 0.83 | 7.15 | 0.178 | 6.67 | BCC+HCP+IM | SS+IM | [59] |
| AlCrFeTI | -30.27 | 0.49 | 5.74 | 0.313 | 4.5 | BCC+IM | SS+IM | [61] |
| (CoCr)80Ni20 | -3.55 | 4.76 | 1.54 | 3.660 | 8 | FCC+HCP | MSS | [62] |
| (CoCr)76.9Ni23.1 | -3.76 | 4.54 | 1.53 | 3.773 | 8.0769 | FCC+HCP | MSS | [62] |
| (CoCr)74.1Ni25.9 | -3.94 | 4.37 | 1.52 | 3.870 | 8.1481 | FCC+HCP | MSS | [62] |
| (CoCr)71.4Ni28.6 | -4.08 | 4.24 | 1.51 | 3.955 | 8.2142 | FCC | SSS | [62] |
| (CoCr)69Ni31 | -4.19 | 4.12 | 1.50 | 4.031 | 8.2758 | FCC | SSS | [62] |
| Cr26Fe24Al50 | -21.28 | 0.59 | 5.76 | 0.260 | 4.98 | BCC+FCC | MSS | [63] |
| Fe40Co30Ni30 | -1.56 | 10.26 | 0.39 | 59.317 | 8.9 | FCC | SSS | [64] |
| Fe47.05Co32.52Ni20.43 | -1.35 | 11.48 | 0.39 | 54.87 | 8.7338 | BCC | SSS | [65] |
| Zr50Ti35Nb15 | 1.44 | 12.40 | 4.23 | 0.463 | 4.15 | BCC | SSS | [66] |
| Fe30Co40Ni30 | -1.56 | 10.23 | 0.36 | 67.683 | 9 | FCC | SSS | [67] |
| Fe40Mn40Co10Cr10 | -0.61 | 27.96 | 4.06 | 0.599 | 7.5 | FCC | SSS | [69] |
| FeAlCrV | -14.6 | 1.40 | 4.87 | 0.485 | 5.5 | BCC+FCC+IM | SS+IM | [70] |
| FeAlCrMo | -10.18 | 2.21 | 5.32 | 0.406 | 5.75 | BCC+FCC+IM | SS+IM | [70] |
| AlFeTiV | -25.91 | 0.76 | 5.83 | 0.338 | 5 | FCC+BCC | MSS | [71] |
| CuZrAl | -38.89 | 0.34 | 9.09 | 0.110 | 6 | FCC+IM | SS+IM | [72] |
| CuZrAlTi | -34.25 | 0.66 | 6.37 | 0.283 | 5.25 | FCC+IM | SS+IM | [72] |
| MoNbTaV | -3.11 | 10.29 | 3.56 | 0.907 | 5.25 | BCC | SSS | [73] |
| MoRhRu | -12.44 | 1.89 | 2.07 | 2.111 | 7.67 | HCP | SSS | [88] |
| (CoFeNi)92.3Si7.7 | -9.87 | 1.90 | 1.98 | 2.725 | 8.615 | FCC | SSS | [89] |
| (CoFeNi)85.7Si14.3 | -16.24 | 1.21 | 2.53 | 1.74 | 8.286 | FCC+IM | SS+IM | [89] |
| (CoFeNi)80Si20 | -20.9 | 0.96 | 3.22 | 1.105 | 8 | FCC+IM | SS+IM | [89] |
| AlCuNi | -17.56 | 0.69 | 5.96 | 0.256 | 8 | FCC+B2 | SS+IM | [90] |
| Al31.25Li15.6Mg31.25Sn6.3Zn15.6 | -3.62 | 2.68 | 6.10 | 0.330 | 3.843 | FCC+IM | SS+IM | [91] |
| NbTaTiV | -0.08 | 387.9 | 3.60 | 0.885 | 4.75 | BCC | SSS | [92] |
| NbTiVZr | -0.15 | 168.7 | 6 | 0.319 | 4.5 | BCC | SSS | [93] |
| Nb20Ti20V40Zr20 | -1.11 | 22.35 | 6.42 | 0.268 | 4.6 | 3 BCC | MSS | [93] |
| MoNbTaW | -6.55 | 5.55 | 2.27 | 2.228 | 5.5 | BCC | SSS | [94] |
| VNbTi | -0.32 | 66.41 | 3.95 | 0.583 | 4.667 | BCC | SSS | [95] |
| Cr12Ni12Mn12Fe64 | -1.56 | 10.14 | 8.45 | 1.355 | 7.88 | FCC | SSS | [96] |
| Cr12Ni12Mn16Fe60 | -1.59 | 10.41 | 9.42 | 1.43 | 7.84 | FCC | SSS | [96] |
| Cr12Ni12Mn20Fe66 | -1.63 | 10.52 | 10.16 | 1.49 | 7.8 | FCC | SSS | [96] |
| Nb31Ti34Zr26Al6V3 | -7.33 | 3.35 | 4.3 | 0.6 | 4.28 | BCC | SSS | [97] |
| Nb31Ti32Zr26Al6V5 | -7.45 | 3.41 | 4.51 | 0.56 | 4.3 | BCC | SSS | [97] |
| Nb31Ti30Zr26Al6V7 | -7.57 | 3.45 | 4.72 | 0.53 | 4.32 | BCC | SSS | [97] |
| Nb31Ti28Zr26Al6V9 | -7.68 | 3.47 | 4.91 | 0.5 | 4.34 | BCC | SSS | [97] |
| Nb31Ti26Zr26Al6V11 | -7.78 | 3.48 | 5.09 | 0.47 | 4.36 | BCC | SSS | [97] |
| MoReRu | -9.79 | 2.78 | 1.78 | 2.857 | 7 | HCP | SSS | [98] |
| Ti10Fe30Co30Ni30 | -10.26 | 1.90 | 5.11 | 1.697 | 8.5 | FCC+B2+L12 | SS+IM | [99] |
| (NiCoCr)92Al6Ta2 | -11.88 | 1.51 | 4.02 | 0.683 | 7.94 | FCC+IM | SS+IM | [100] |
| (CoCrNi)91Al9 | -13.1 | 1.49 | 4 | 0.679 | 7.846 | FCC+IM | SS+IM | [101] |
| (VCoNi)91Al9 | -21.49 | 0.91 | 4.75 | 0.48 | 7.545 | FCC+BCC | MSS | [102] |
| (VCr)33.4(CoNi)66.6 | -9.82 | 2.13 | 2.92 | 1.29 | 7.666 | FCC+HCP | MSS | [103] |
| (CoCrNi)96.8Ta3.2 | -7.17 | 2.7 | 3.22 | 0.96 | 8.22 | FCC+laves | SS+IM | [104] |
| CoNiV | -14.19 | 1.21 | 3.67 | 0.676 | 8 | FCC | SSS | [105] |
| (CoNiV)97Al3 | -16.79 | 1.10 | 4.09 | 0.549 | 7.85 | FCC | SSS | [105] |
| (CoNiV)95Al5 | -18.42 | 1.03 | 4.33 | 0.549 | 7.75 | FCC+B2 | SS+IM | [105] |
| (CoFe)70.6Al17.6Cr11.8 | -15.56 | 1.16 | 5.10 | 0.412 | 7.235 | BCC+ L21 | SS+IM | [106] |
| Fe50Mn25Cr15Ni10 | -1.49 | 12.05 | 3.64 | 0.757 | 7.65 | FCC | SSS | [107] |
| Fe50Mn25Cr15(NiCo)10 | -1.18 | 16.13 | 3.64 | 0.801 | 7.6 | FCC+HCP | MSS | [107] |
| Fe50Mn25Cr15Co10 | -0.86 | 20.88 | 3.64 | 0.757 | 7.55 | FCC+HCP | MSS | [107] |
| VNbTiSi | -38.83 | 0.63 | 8.68 | 0.152 | 4.5 | BCC+IM | SS+IM | [108] |
| (CoCrNi)94Al3Ti3 | -10.28 | 1.96 | 3.78 | 0.756 | 8.043 | FCC+ L12 | SS+IM | [109] |
| V47Fe11Ti30Cr10La2 | -4.42 | 4.88 | 7.33 | 0.196 | 5.09 | BCC+laves | SS+IM | [111] |
| V47Fe11Ti30Cr10Ce2 | -4.59 | 4.70 | 6.98 | 0.215 | 5.11 | BCC+laves | SS+IM | [111] |
| V47Fe11Ti30Cr10Y2 | -4.82 | 4.5 | 6.92 | 0.219 | 5.09 | BCC+laves | SS+IM | [111] |
| V47Fe11Ti30Cr10Sc2 | -5.53 | 3.92 | 5.89 | 0.303 | 5.09 | BCC+laves | SS+IM | [111] |
| CoNiFe | -1.03 | 15.67 | 0.38 | 2 | 8.991 | FCC | SSS | [112] |
| Fe42.8Cr28.6(NiCu)28.6 | 3.29 | 5.93 | 1.19 | 2 | 8.142 | FCC+BCC | MSS | [113] |
| Fe42.1Cr28.1(NiCu)28Al1.8 | 1.71 | 11.87 | 2.02 | 2 | 8.05 | FCC+BCC | MSS | [113] |
| Fe41.4Cr27.6(NiCu)27.6Al3.4 | 0.25 | 84.85 | 2.56 | 1.742 | 7.965 | FCC+BCC | MSS | [113] |
| Fe40Cr26.7(NiCu)26.6Al6.7 | -2.41 | 8.82 | 3.31 | 1.084 | 7.8 | FCC+BCC | MSS | [113] |
| (FeNi)60(AlCr)40 | -18.75 | 1.02 | 5.24 | 0.413 | 7.2 | BCC+B2 | SS+IM | [114] |
| Co35Cr30Ni27Al4Ti4 | -11.76 | 1.75 | 4.23 | 0.621 | 7.93 | FCC+ L12 | SS+IM | [115] |
| ScGdHo | 0.71 | 22.14 | 3.61 | 0.697 | 8.666 | HCP | SSS | [116] |
| (TiNb)75Zr25 | 2.51 | 8.22 | 3.74 | 0.64 | 4.375 | BCC | SSS | [117] |
| (TiZr)75Nb25 | 2.1 | 9.50 | 4.14 | 0.523 | 4.25 | BCC | SSS | [117] |
| Fe20Cr20Ni30Al30 | -23.97 | 0.75 | 5.87 | 0.328 | 6.7 | BCC+B2 | SS+IM | [118] |
| (TiZr)90Nb7Sn3 | -4.52 | 3.79 | 4.20 | 0.474 | 4.07 | BCC | SSS | [119] |
| (TiZr)90Nb5Sn5 | -8.06 | 2.09 | 4.18 | 0.484 | 4.05 | BCC | SSS | [119] |
| (TiZr)90Nb3Sn7 | -11.56 | 1.41 | 4.15 | 0.486 | 4.03 | BCC | SSS | [119] |
| (NbTiZr)96.8(MoTa)3.2 | 2.14 | 10.97 | 4.11 | 0.602 | 4.3709 | BCC | SSS | [120] |
| (CrCoNi)83.3Mo16.7 | -5.67 | 4.12 | 4.18 | 0.649 | 7.944 | FCC+laves+ σ | SS+IM | [121] |
| (CrTaTi)89.6Al10.4 | -15.92 | 1.59 | 5.7 | 0.337 | 4.791 | BCC+IM | SS+IM | [122] |
| MoNbV | -2.94 | 8.11 | 3.49 | 0.746 | 5.333 | BCC | SSS | [123] |
| MoNbVTi | -2.45 | 11.50 | 3.56 | 0.907 | 5 | BCC | SSS | [123] |
| Fe65Cr15(CoNi)12Si8 | -10.09 | 1.68 | 2.027 | 2 | 7.56 | BCC+FCC | MSS | [124] |
| (CrFeNi)88.2Nb11.8 | -10.55 | 2.1 | 5.224 | 0.405 | 7.647 | FCC+laves | SS+IM | [125] |
| (CrFeNi)78.1Nb21.1 | -14.22 | 1.68 | 6.434 | 0.277 | 7.368 | FCC+laves | SS+IM | [125] |
| (CrFeNi)85.7Nb14.3 | -11.66 | 1.95 | 5.624 | 0.355 | 7.5714 | FCC+laves | SS+IM | [125] |
| (CrFeNi)83.3Nb16.7 | -12.63 | 1.84 | 5.947 | 0.321 | 7.5 | FCC+laves | SS+IM | [125] |
| (CrFeNi)81.1Nb18.9 | -13.48 | 1.75 | 6.213 | 0.296 | 7.4324 | FCC+laves | SS+IM | [125] |
| (CoNi)74V16Mo10 | -9.43 | 2.14 | 4.195 | 0.594 | 8.43 | FCC+ µ | SS+IM | [126] |

Chart, scatter chart

Description automatically generated

**Figure F1:** Scatter plot of SSS, MSS and SS+IM in vs. binary feature space

**Table S3:** Dataset used for phase prediction in the case study section (Section 5)

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Medium entropy alloy composition** | **(KJ/mol)** |  |  | **VEC** | **Phase name** | **Phase category** | **Reference** |
| Fe25Cr50V25 | -3.46 | 2.52 | 1.36 | 6.25 | Dual BCC | SS | [127] |
| Fe24.4Cr48.8V24.4W2.4 | -3.27 | 2.81 | 1.18 | 6.24 | Dual BCC | SS | [127] |
| Co35Ni36Cr23Mo6 | -4.68 | 4.46 | 0.518 | 7.29 | FCC | SS | [128] |
| Fe44.4Co31.7Ni19Nb4.8 | -4.74 | 3.64 | 0.741 | 8.55 | FCC+BCC | SS | [129] |
| Fe46.7Co33.3Ni20 | -0.98 | 0.38 | 54.88 | 8.73 | BCC | SS | [129] |
| Co50Mn33.3Ge16.7 | -16.65 | 4.84 | 0.357 | 7.5 | HCP | SS | [130] |
| Al15Nb40Ti40V5 | -21.03 | 3.16 | 1.07 | 4 | BCC+B2 | SS+IM | [131] |
| Al20Nb40Ti40 | -21.25 | 1.09 | 7.32 | 4.2 | BCC+B2 | SS+IM | [131] |
| TiZrMo | -4.32 | 5.56 | 0.29 | 4.67 | Dual BCC | SS | [132] |
| TiVMo | -2.29 | 3.5 | 0.74 | 5 | BCC | SS | [132] |
| TiVZrMo | -3.75 | 6.45 | 0.27 | 4.75 | Dual BCC+Laves | SS+IM | [132] |
| Fe16.7Cr19.7Ni46.8Al16.7 | -18.42 | 5.01 | 0.42 | 7.7 | BCC+FCC+B2 | SS+IM | [133] |
| Fe24.5Cr16.8Ni41.9Al16.8 | -17.74 | 5.01 | 0.43 | 7.6 | BCC+FCC+B2 | SS+IM | [133] |
| Fe40Ni25Mn25Cu10 | 0.25 | 3.77 | 0.752 | 8.55 | Dual FCC | SS | Present study |
| Ni35Zn30Fe20Mn15 | -11.95 | 4.45 | 0.562 | 9.75 | Dual FCC | SS | Present study |
| Ca60Mg15Cu15Zn10 | -10.33 | 16.15 | 0.035 | 4.35 | AM | AM | Present study |

**Table S4:** Mixing entropy (), mixing enthalpy (), , , phase name and category for HEAs. Dataset used for ternary classification of phases in HEA (SS, SS+IM, AM) [25,27,48]

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **High entropy alloy composition** | **(J/K)** | **(KJ/mol)** |  |  | **Phase category** |
| Al15.79(HfNbTiZr)84.21 | 13.33 | -15.64 | 4.97 | 0.540 | SS |
| AlCoCrFeNi | 13.38 | -12.32 | 5.25 | 0.485 | SS |
| (AlCrFeNi)95.24Mo4.76 | 12.57 | -12.65 | 6.20 | 0.327 | SS |
| (AlCrFeNi)88.89Mo11.11 | 13.15 | -11.85 | 6.11 | 0.352 | SS |
| FeCrCoMnNi | 13.38 | -4.16 | 3.27 | 1.252 | SS |
| Fe20Co27Ni13Cr20Mn20 | 13.17 | -3.76 | 3.26 | 1.242 | SS |
| Fe20Co23Ni17Cr20Mn20 | 13.1 | -3.88 | 2.59 | 1.953 | SS |
| (HfNbTi)66.67(VSiMo)33.33 | 14.54 | -31.11 | 9.44 | 0.163 | SS |
| TiZrHfNbCu | 13.38 | -5.76 | 7.79 | 0.220 | SS |
| Al5(HfNbTiZr)95 | 12.6 | -6.22 | 4.92 | 0.520 | SS |
| (CoCrFeNi)95.24Ti4.76 | 12.57 | -7.34 | 3.66 | 0.939 | SS |
| Al11.11(MoNbTiV)88.89 | 13.15 | -7.01 | 3.93 | 0.850 | SS |
| Al13.04(MoTaTiV)86.96 | 13.24 | -8.01 | 3.90 | 0.868 | SS |
| Al27.27(MoNbTiV)72,73 | 13.25 | -13.81 | 3.67 | 0.984 | SS |
| Cr11.11(AlNbTiV)88.89 | 13.15 | -15.40 | 5.23 | 0.480 | SS |
| V10Cr15Mn5Fe35Co10Ni25 | 13.38 | -6.26 | 2.40 | 2.316 | SS |
| AlCrMoNbTi | 13.38 | -13.6 | 4.87 | 0.564 | SS |
| Al20Nb30Ta10Ti30Zr10 | 12.51 | -15.12 | 3.07 | 1.327 | SS |
| Al8Hf12(NbTaTiZr)80 | 14.5 | -6.33 | 4.11 | 0.858 | SS |
| Mo31.26Nb20.83Ti20.83V6.25Zr20.83 | 12.61 | -3.48 | 6.37 | 0.311 | SS |
| (MoNbTaW)84.21Ti15.79 | 13.33 | -2.70 | 3.75 | 0.950 | SS |
| AlNbTaTiV | 13.38 | -13.44 | 3.16 | 1.340 | SS |
| Hf12.5Mo12.5(NbTiZr)75 | 12.97 | -0.25 | 5.73 | 0.395 | SS |
| (AlCoCrFeNi)98.04Mo1.96 | 13.92 | -12.13 | 5.30 | 0.496 | SS |
| Mo11.11(NbTiVZr)88.89 | 13.15 | -1.77 | 6.97 | 0.271 | SS |
| Mo17.5Nb25Ti25V7.5Zr25 | 12.8 | -1.82 | 6.33 | 0.319 | SS |
| Mo6.97(NbTiVZr)93.03 | 13.31 | -2.20 | 6.93 | 0.277 | SS |
| (AlCoCrFeNi)98.04Nb1.96 | 13.92 | -13.31 | 5.92 | 0.397 | SS |
| (AlCoCrFeNi)96.15Si3.85 | 14.22 | -16.39 | 6.02 | 0.393 | SS |
| (AlCoCrFeNi)92.6Si7.4 | 14.59 | -19.83 | 6.21 | 0.378 | SS |
| (AlCoCrFeNi)89.29Si10.71 | 14.78 | -22.75 | 6.37 | 0.364 | SS |
| (CoCrCuFeNi)90.9Ti9.1 | 14.7 | -17.05 | 4.82 | 0.632 | SS |
| Al11.11(CoCrFeNi)88.89 | 13.15 | -9.09 | 4.22 | 0.738 | SS |
| AlCrFeMnNi | 13.38 | -12.48 | 5.83 | 0.394 | SS |
| CoCrCuFeNi | 13.38 | 3.2 | 1.07 | 11.687 | SS |
| (CoCrCuFeNi)96Nb4 | 14.24 | -14.24 | 2.92 | 1.674 | SS |
| AlHfNbTaTiZr | 14.9 | -14.77 | 4.90 | 0.620 | SS |
| Mo12.2Nb24.4Hf12.2Zr24.4Ti24.4Si2.4 | 13.6 | -6.47 | 6.69 | 0.304 | SS |
| Al9.1(CoCrCuFeNi)90.9 | 14.7 | -1.52 | 3.82 | 1.007 | SS |
| AlCoCrCuFeNi | 14.9 | -4.78 | 4.82 | 0.641 | SS |
| Al28.57(CoCrCuFeNi)71.43 | 14.53 | -8.65 | 5.71 | 0.446 | SS |
| MoNbHfZrTi | 13.38 | -3.2 | 6.10 | 0.360 | SS |
| MoNbTaVW | 13.38 | -4.64 | 3.21 | 1.299 | SS |
| Hf23.26Mo11.62Nb23.26Ti23.26V11.62Si6.98 | 14.17 | -16.36 | 7.88 | 0.228 | SS |
| CrMoNbTiV | 13.38 | -4.32 | 5.62 | 0.424 | SS |
| MoNbTaTiV | 13.38 | -2.56 | 3.34 | 1.199 | SS |
| HfNbTaTiZr | 13.38 | 2.72 | 4.01 | 0.832 | SS |
| (ZrTiHf)75V12.5Nb12.5 | 12.97 | 0.43 | 6.44 | 0.313 | SS |
| Zr28.57(TiHfV)42.86Nb28.57 | 12.89 | 1.46 | 6.80 | 0.279 | SS |
| (ZrTiHf)75Nb12.5Mo12.5 | 12.97 | -2.12 | 5.70 | 0.399 | SS |
| (ZrTiHf)75Nb12.5Ta12.5 | 12.97 | 0.87 | 4.86 | 0.549 | SS |
| Al5.66(HfNbTaTiZr)94.34 | 12.83 | -5.04 | 4.75 | 0.568 | SS |
| Al9.1(HfNbTaTiZr)90.9 | 13.15 | -8.98 | 4.70 | 0.596 | SS |
| Al13.04(HfNbTaTiZr)86.96 | 14.86 | -11.55 | 4.23 | 0.830 | SS |
| AlCoCuFeNi | 13.38 | -4.97 | 5.61 | 0.425 | SS |
| AlNbTiVZr | 13.38 | -17.44 | 5.53 | 0.438 | SS |
| (AlCoCrFeNi)96.16V3.84 | 14.22 | -13.07 | 5.68 | 0.441 | SS |
| (AlCoCrFeNi)90.9V9.1 | 14.7 | -13.95 | 5.54 | 0.478 | SS |
| (AlCoCrFeNi)86.2V13.8 | 14.87 | -14.57 | 5.42 | 0.507 | SS |
| AlCoCrFeNiV | 14.9 | -14.88 | 5.33 | 0.524 | SS |
| Al20(CoCrFeNi)66.67Ti13.33 | 14.84 | -20.86 | 7.12 | 0.293 | SS |
| Al11.11(HfNbTiZr)88.89 | 13.15 | -10.96 | 4.96 | 0.535 | SS |
| Al6.52(CoCrFeNi)86.96Cu6.52 | 13.99 | -4.38 | 3.65 | 1.052 | SS |
| CrCoFeNiMn | 13.38 | -4.16 | 0.92 | 15.808 | SS |
| (TiZrHfMo)95.24Cr4.76 | 12.57 | -4.44 | 7.25 | 0.239 | SS |
| Cr26Mn20Fe20Co20Ni14 | 13.23 | -3.72 | 3.26 | 1.243 | SS |
| HfNbTaTiZrW | 14.9 | -3.22 | 5.72 | 0.455 | SS |
| HfNbTaTiZrMoW | 16.18 | -2.93 | 6.02 | 0.446 | SS |
| Ti38.1Zr19.05Hf9.52V19.05Nb14.28 | 12.48 | 0.10 | 6.56 | 0.290 | SS |
| Ti36.36(ZrVNb)54.54Hf9.1 | 12.6 | 0.52 | 6.44 | 0.304 | SS |
| ZrTiHfCuNiFe | 14.9 | -24.77 | 10.92 | 0.125 | SS |
| AlCrFeCoNi | 13.38 | -12.32 | 5.78 | 0.400 | SS |
| (CoCrFeNi)95.24Mo4.76 | 12.57 | -4.04 | 2.51 | 1.995 | SS |
| (CrMnFeV)95.24Cu4.76 | 12.57 | 2.67 | 3.47 | 1.046 | SS |
| NbMoTaWVTi | 14.9 | -4.22 | 3.58 | 1.165 | SS |
| Al6.25Fe31.25(MnNiCr)62.5 | 12.61 | -6.55 | 4.55 | 0.610 | SS |
| MoNbTaTiZr | 13.38 | -1.76 | 5.46 | 0.448 | SS |
| (CoCrMoNb)90.9Ti9.1 | 13.01 | -12.76 | 6.24 | 0.335 | SS |
| Al8Co17Cr17Cu8Fe17Ni33 | 13.92 | -5.12 | 3.99 | 0.876 | SS |
| Al9.1(CoCrFeMnNi)90.9 | 16.01 | -2.65 | 4.43 | 0.817 | SS |
| (CoCrFeNi)94.12V5.88 | 12.71 | -5.59 | 1.34 | 7.132 | SS |
| (CoCrFeMnNi)99C1 | 13.71 | -6.12 | 5.08 | 0.530 | SS |
| (FeMnNiCoCr)99.8C0.2 | 13.47 | -4.55 | 3.71 | 0.981 | SS |
| (FeMnNiCoCr)99.5C0.5 | 13.58 | -5.14 | 4.27 | 0.744 | SS |
| (FeMnNiCoCr)99.2C0.8 | 13.66 | -5.72 | 4.77 | 0.600 | SS |
| (AlCoCrFe)48.78Ni51.22 | 12.91 | -11.94 | 5.38 | 0.446 | SS |
| Al20Mo10Nb20Ta10Ti20Zr20 | 14.53 | -16.84 | 4.34 | 0.771 | SS |
| Al6Nb20Ta16Ti28V4Zr26 | 13.46 | -4.86 | 4.50 | 0.665 | SS |
| Al10Nb20Ta16Ti30V4Zr20 | 13.78 | -8.62 | 4.23 | 0.770 | SS |
| Mo27.27(NbHfZrTi)72.73 | 13.25 | -2.64 | 6.34 | 0.330 | SS |
| (FeCoNiCrMn)98Al2 | 13.93 | -5.26 | 3.70 | 1.016 | SS |
| (FeCoNiCrMn)96Al4 | 14.24 | -6.32 | 4.07 | 0.860 | SS |
| (FeCoNiCrMn)93Al7 | 14.55 | -7.81 | 4.53 | 0.708 | SS |
| (FeCoNiCrMn)92Al8 | 14.63 | -8.29 | 4.67 | 0.671 | SS |
| (FeCoNiCrMn)91Al9 | 14.69 | -8.75 | 4.80 | 0.639 | SS |
| (FeCoNiCrMn)90Al10 | 14.75 | -9.20 | 4.92 | 0.610 | SS |
| (FeCoNiCrMn)89Al11 | 14.79 | -9.63 | 5.03 | 0.585 | SS |
| (TiZrNbV)70.18Mo29.82 | 13.16 | -4.70 | 6.67 | 0.296 | SS |
| (TiZrNbV)66.67Mo33.33 | 12.98 | -4.77 | 6.58 | 0.300 | SS |
| CrFeCoNiCu | 13.25 | 2.31 | 1.00 | 13.287 | SS |
| Cu4.35(AlCoCrFeNi)86.95Ti8.7 | 15.55 | -15.50 | 6.58 | 0.359 | SS |
| Cu8.33(AlCoCrFeNi)83.34Ti8.33 | 15.86 | -13.41 | 6.46 | 0.380 | SS |
| AlCrFeCoNiCu | 14.9 | -4.77 | 5.28 | 0.534 | SS |
| AlCrFeCoNiCuTi | 16.18 | -13.79 | 6.78 | 0.352 | SS |
| AlCrFeCoNiCuV | 16.18 | -7.75 | 4.95 | 0.659 | SS |
| Co25Ni25Fe25Al7.5Cu17.5 | 12.8 | 0.82 | 3.87 | 0.853 | SS |
| HfMoTaTiZr | 13.38 | -1.92 | 6.09 | 0.361 | SS |
| HfMoNbTaZr | 13.38 | -1.12 | 6.30 | 0.337 | SS |
| HfMoNbTaTi | 13.38 | 2.72 | 4.99 | 0.536 | SS |
| Ni18.5Fe18.5Cr18.5Co26Mn18.5 | 13.29 | -4.11 | 3.17 | 1.326 | SS |
| Ni27.27Co27.27(CrFe)36.36Ti9.1 | 12.86 | -10.74 | 4.89 | 0.539 | SS |
| (CoNiFeCr)93Mo7 | 12.83 | -4.45 | 3.88 | 0.851 | SS |
| Cr30Cu10(MnFeNi)60 | 12.95 | 0.08 | 3.25 | 1.227 | SS |
| Cr25Cu15(MnFeNi)60 | 13.28 | 1.52 | 3.23 | 1.277 | SS |
| CrCoCuFeNi | 13.38 | 3.2 | 1.03 | 12.534 | SS |
| CoCrCuFeMn | 13.38 | 4.16 | 3.15 | 1.351 | SS |
| (TiZrNbTa)95Mo5 | 12.6 | 1.26 | 3.96 | 0.803 | SS |
| (TiZrNbTa)90Mo10 | 13.08 | 0.13 | 4.13 | 0.767 | SS |
| (TiZrNbTa)85Mo15 | 13.31 | -0.87 | 4.27 | 0.730 | SS |
| AlCoCrCuMnFe | 14.9 | -3.77 | 5.34 | 0.523 | SS |
| (TiZrNbMo)95.24V4.76 | 12.71 | -2.60 | 6.32 | 0.319 | SS |
| (TiZrNbMo)88.89V11.11 | 13.15 | -2.66 | 6.55 | 0.306 | SS |
| (TiZrNbMo)84.21V15.79 | 13.33 | -2.70 | 6.73 | 0.295 | SS |
| TiZrNbMoV | 13.38 | -2.72 | 6.85 | 0.285 | SS |
| (TiZrNbMo)72.73V27.27 | 13.25 | -2.71 | 7.01 | 0.270 | SS |
| (TiZrNbMo)66.67V33.33 | 12.98 | -2.66 | 7.07 | 0.260 | SS |
| Al6.67Cr22.22Fe33.33Mn22.22Ni11.11Ti4.45 | 13.28 | -7.67 | 5.40 | 0.456 | SS |
| Al22.5Ti22.5Ni20Cu20Fe15 | 13.3 | -19.95 | 7.17 | 0.259 | SS |
| AlTiNiCuFe | 13.38 | -17.6 | 7.16 | 0.261 | SS |
| Al10(CoCrFeNi)80Ti10 | 14.53 | -15.52 | 6.25 | 0.372 | SS |
| Al16(CoCrFeNi)80Ti4 | 14.84 | -21.97 | 7.32 | 0.277 | SS |
| (CoCrFeNiMn)99.8C0.2 | 13.47 | -4.55 | 3.70 | 0.982 | SS |
| Al6.98(CoCrFeNi)93.02 | 12.83 | -7.27 | 3.49 | 1.053 | SS |
| Al7(HfNbTiZr)93 | 12.83 | -8.52 | 4.94 | 0.527 | SS |
| (MoHfZrTi)88.89Nb11.11 | 13.15 | -3.35 | 6.25 | 0.336 | SS |
| (MoHfZrTi)72.73Nb27.27 | 13.25 | -3.04 | 5.94 | 0.375 | SS |
| (MoNbHfZr)88.89Ti11.11 | 13.15 | -3.75 | 6.39 | 0.322 | SS |
| (MoNbHfZr)72.73Ti27.27 | 13.25 | -2.77 | 5.84 | 0.388 | SS |
| (MoNbHfTi)88.89Zr11.11 | 13.15 | -2.76 | 5.86 | 0.382 | SS |
| (MoNbHfTi)72.73Zr27.27 | 13.25 | -3.43 | 6.19 | 0.346 | SS |
| (MoNbZrTi)88.89Hf11.11 | 13.15 | -3.95 | 6.10 | 0.354 | SS |
| (MoNbZrTi)72.73Hf27.27 | 13.25 | -2.64 | 6.04 | 0.363 | SS |
| AlHfNbTiZr | 13.38 | -19.36 | 4.97 | 0.542 | SS |
| Al23.8(HfNbTiZr)76.2 | 13.35 | -22.31 | 4.96 | 0.543 | SS |
| Al27.27(HfNbTiZr)72.73 | 13.25 | -24.66 | 4.94 | 0.544 | SS |
| Mo28.26(NbTiZr)65.22V6.52 | 12.72 | -3.19 | 6.38 | 0.313 | SS |
| Mo24.53(NbTiVZr)75.47 | 13.33 | -3.10 | 6.77 | 0.290 | SS |
| (MoNbTaW)94.12Ti5.88 | 12.71 | -6.14 | 2.49 | 2.057 | SS |
| (MoNbTaW)88.89Ti11.11 | 13.15 | -2.86 | 3.69 | 0.967 | SS |
| (MoNbTiZr)93.02V6.98 | 12.83 | -2.61 | 6.37 | 0.316 | SS |
| MoNbTiVZr | 13.38 | -2.72 | 5.77 | 0.402 | SS |
| (AlCoCrFeNi)90.9Ti9.1 | 14.7 | -17.92 | 6.12 | 0.392 | SS |
| AlCoCrFeNiTi | 14.9 | -21.56 | 6.58 | 0.344 | SS |
| (CoCrFeMnNi)95.24V4.76 | 14.34 | -5.29 | 3.29 | 1.327 | SS |
| (CoCrFeMnNi)90.9V9.1 | 14.7 | -6.21 | 3.30 | 1.354 | SS |
| (CoCrFeNi)95.24W4.76 | 12.57 | -3.53 | 2.07 | 2.946 | SS |
| Al10.71(CrCuFe)53.58Ni35.71 | 12.72 | -7.15 | 4.12 | 0.749 | SS |
| Al16.67(CrCuFeNi)83.33 | 13.35 | -8.47 | 4.73 | 0.597 | SS |
| (AlCrCuFe)66.67Ni33.33 | 12.98 | -11.45 | 4.86 | 0.550 | SS |
| Al19.35(CrCuFe)48.39Ni32.26 | 13.02 | -13.16 | 5.11 | 0.499 | SS |
| Al5.66(CrCuFeMnNi)94.34 | 14.43 | -0.81 | 4.03 | 0.888 | SS |
| Al9.1(CrCuFeMnNi)90.9 | 14.7 | -3.37 | 4.38 | 0.766 | SS |
| Al13.8(CrCuFeMnNi)86.2 | 14.87 | -6.55 | 4.76 | 0.656 | SS |
| Al12.7(CrCuFeNi)63.5Mn23.8 | 14.74 | -5.87 | 4.02 | 0.912 | SS |
| Al12.7(CrFeMnNi)63.5Cu23.8 | 14.74 | -4.36 | 4.61 | 0.694 | SS |
| CoCrFeNiPd | 13.38 | -5.62 | 3.54 | 1.069 | SS |
| (CoCrFeNi)66.67Pd33.33 | 12.98 | -6.16 | 4.03 | 0.799 | SS |
| Al6Nb20Ta16Ti28V4Zr26 | 13.46 | -5.52 | 4.41 | 0.692 | SS |
| Al10Nb20Ta16Ti30V4Zr20 | 13.78 | -10.27 | 4.15 | 0.800 | SS |
| Al6Nb20Ta20Ti28Zr26 | 12.63 | -5.29 | 3.94 | 0.814 | SS |
| Al5.88(NbTaTiV)94.12 | 12.71 | -7.15 | 3.50 | 1.038 | SS |
| (CoCrMoNb)95.24Ti4.76 | 12.57 | -12.3356 | 6.05 | 0.343 | SS+IM |
| (CoCrMoNb)88.89Ti11.11 | 13.15 | -12.9383 | 6.31 | 0.330 | SS+IM |
| CoCrMoNbTi | 13.38 | -13.44 | 6.53 | 0.313 | SS+IM |
| (AlCoCrFeNi)76.93C23.07 | 14.79 | -15.3846 | 5.15 | 0.558 | SS+IM |
| (CoCrFeNi)95.1Nb4.9 | 12.59 | -7.0248 | 3.15 | 1.272 | SS+IM |
| (CoCrFeNi)92.83Nb7.17 | 12.84 | -8.385 | 3.73 | 0.924 | SS+IM |
| (CoCrFeNi)90.67Nb9.33 | 13.03 | -9.6859 | 4.21 | 0.737 | SS+IM |
| (CoCrFeMnNi)86.96V13.04 | 14.86 | -6.9565 | 3.29 | 1.369 | SS+IM |
| CoCrFeMnNiV | 14.9 | -7.5556 | 3.29 | 1.378 | SS+IM |
| (AlCrFeNi)83.33Mo16.67 | 13.35 | -11.1458 | 6.02 | 0.369 | SS+IM |
| (VCrFe)78.96Ta10.52W10.52 | 12.7 | -5.6288 | 4.82 | 0.546 | SS+IM |
| (NbCrTiZr)75(MoTa)25 | 14.53 | -4.92 | 7.13 | 0.286 | SS+IM |
| Nb42Mo20Ti13Cr12V12Ta1 | 12.52 | -4.2436 | 4.59 | 0.594 | SS+IM |
| (AlCoCrFeNi)96.15Ti3.85 | 14.22 | -14.8521 | 6.23 | 0.366 | SS+IM |
| (CoCrCuFeNi)92Nb8 | 14.63 | -15.3853 | 3.89 | 0.965 | SS+IM |
| (CoCrCuFeNi)88Nb12 | 14.83 | -16.3722 | 4.59 | 0.704 | SS+IM |
| (AlCoCrFeNi)92.6Ti7.4 | 14.59 | -16.9822 | 6.58 | 0.337 | SS+IM |
| CrMoNbTaVW | 14.9 | -4.89 | 4.78 | 0.652 | SS+IM |
| AlCoCrFeNi | 13.38 | -12.32 | 5.25 | 0.485 | SS+IM |
| CrMoNbTiW | 13.38 | -7.04 | 7.65 | 0.228 | SS+IM |
| Fe34Cr34Ni14Al14Co4 | 12.63 | -7.5744 | 4.43 | 0.644 | SS+IM |
| (AlNbTiV)94.12Zr5.88 | 12.71 | -17.3841 | 4.97 | 0.515 | SS+IM |
| (AlNbTiV)88.89Zr11.11 | 13.15 | -18.1728 | 5.61 | 0.418 | SS+IM |
| Al12(HfNbTiZr)88 | 13.19 | -13.8336 | 4.96 | 0.536 | SS+IM |
| Al3.7(CrFeCo)55.57Ni37.03Cu3.7 | 12.88 | -4.5322 | 2.82 | 1.615 | SS+IM |
| Al10Co25Cr8Fe15Ni36Ti6 | 13.3 | -13.9748 | 5.66 | 0.416 | SS+IM |
| Al3.63Co27.27Cr18.19Fe18.19Ni27.27Ti5.45 | 13.37 | -10.0298 | 4.63 | 0.624 | SS+IM |
| Hf12.2Mo12.2(NbTiZr)73.17C2.43 | 13.6 | -6.4723 | 9.45 | 0.152 | SS+IM |
| Mo11.12Nb22.22Hf11.11Zr22.22Ti22.22Si11.11 | 14.43 | -26.0741 | 9.17 | 0.171 | SS+IM |
| HfNbTiVZr | 13.38 | 0.16 | 6.08 | 0.362 | SS+IM |
| CrHfNbTiZr | 13.38 | -4 | 8.63 | 0.180 | SS+IM |
| (CoCrFeNi)83.33V16.67 | 13.35 | -8.2986 | 2.07 | 3.118 | SS+IM |
| (CoCrFeNi)81.63V18.37 | 13.37 | -8.6464 | 2.15 | 2.903 | SS+IM |
| (AlCoCrFeNi)76.93Ti23.07 | 14.79 | -23.91 | 6.84 | 0.316 | SS+IM |
| (CoCrFeNi)88.89W11.11 | 13.15 | -3.2593 | 3.01 | 1.449 | SS+IM |
| CrNbTiVZr | 13.38 | -4.64 | 7.67 | 0.227 | SS+IM |
| (FeCoNiCr)94Ti2Al4 | 13.04 | -7.3763 | 3.71 | 0.949 | SS+IM |
| (AlCoCrFeNi)92.6Mo7.4 | 14.59 | -11.6 | 5.44 | 0.493 | SS+IM |
| (AlCoCrFeNi)90.9Mo9.1 | 14.7 | -11.44 | 5.47 | 0.491 | SS+IM |
| (AlCoCrFeNi)86.2Si13.8 | 14.87 | -25.2319 | 6.50 | 0.352 | SS+IM |
| AlCoCrFeNiSi | 14.9 | -27.3333 | 6.61 | 0.341 | SS+IM |
| CoCrMoNbTi | 13.38 | -13.44 | 6.53 | 0.313 | SS+IM |
| (CoCrFeNi)94.12Nb5.88 | 12.71 | -7.6401 | 3.42 | 1.085 | SS+IM |
| AlCCoCrFeNi | 14.9 | -33.8889 | 16.86 | 0.052 | SS+IM |
| (AlCoCrFeNi)96.15Mo3.85 | 14.22 | -11.95 | 5.35 | 0.497 | SS+IM |
| (AlCoCrFeNi)94.34Mo5.66 | 14.43 | -11.7764 | 5.77 | 0.433 | SS+IM |
| Al13.33(CoCrFeNi)66.67Ti20 | 14.84 | -21.9778 | 7.32 | 0.277 | SS+IM |
| (CoCrFeNi)88.89V11.11 | 13.15 | -7.0123 | 1.76 | 4.256 | SS+IM |
| (CoCrFeNi)85.1V14.9 | 13.31 | -7.9131 | 1.98 | 3.393 | SS+IM |
| Al33.33(CoCrFeNi)66.67 | 12.98 | -15.4444 | 6.68 | 0.291 | SS+IM |
| (AlCoCrFeNi)95.24Nb4.76 | 14.34 | -14.6576 | 6.10 | 0.386 | SS+IM |
| (AlCoCrFeNi)90.9Nb9.1 | 14.7 | -16.5289 | 6.33 | 0.367 | SS+IM |
| Al12.5(CrFeNi)75Co7.5C5 | 13.67 | -17.9925 | 10.00 | 0.137 | SS+IM |
| AlCoCrCuMnTi | 14.9 | -12.8889 | 6.36 | 0.368 | SS+IM |
| Al6.67Cr22.22Fe33.33Mn22.22Ni11.11Si4.45 | 13.28 | -11.356 | 5.07 | 0.517 | SS+IM |
| (AlCoCrFeNi)98.04C1.96 | 13.92 | -15.3479 | 8.01 | 0.217 | SS+IM |
| (AlCoCrFeNi)96.16C3.84 | 14.22 | -18.1361 | 9.67 | 0.152 | SS+IM |
| (AlCoCrFeNi)94.33C5.67 | 14.43 | -20.7049 | 11.02 | 0.119 | SS+IM |
| (AlCoCrFeNi)92.6C7.4 | 14.59 | -23.0727 | 12.17 | 0.099 | SS+IM |
| (AlCoCrFeNi)90.9C9.1 | 14.7 | -25.2562 | 13.17 | 0.085 | SS+IM |
| Al18Cr28Nb18Ti18V18 | 13.23 | -13.6656 | 6.32 | 0.331 | SS+IM |
| Fe22Co20Ni19Cr20Mn12Al7 | 14.41 | -7.5184 | 4.35 | 0.763 | SS+IM |
| AlLiMgZnSn | 13.38 | -6.08 | 5.16 | 0.503 | SS+IM |
| Al17.5Co7.5(CrFeNi)75 | 12.8 | -11.4 | 5.54 | 0.417 | SS+IM |
| (CoCrCuFeNi)84Nb16 | 14.9 | -17.2086 | 5.12 | 0.568 | SS+IM |
| AlCrNbTiV | 13.38 | -14.56 | 5.90 | 0.384 | SS+IM |
| Al40(CuCrFeSi)60 | 12.51 | -15.87 | 8.03 | 0.194 | SS+IM |
| CoCrFeNiV | 13.38 | -8.96 | 2.21 | 2.731 | SS+IM |
| Co20Cr20Fe34Mn20Ni6 | 12.48 | -2.5472 | 3.30 | 1.144 | SS+IM |
| (AlCoCrFe)66.115Mo0.885Ni33 | 13.27 | -11.9445 | 5.42 | 0.451 | SS+IM |
| Al19Co19Cr19Fe24Ni19 | 13.34 | -11.6888 | 5.69 | 0.412 | SS+IM |
| Al17Co17Cr17Fe32Ni17 | 13.05 | -10.4312 | 5.49 | 0.434 | SS+IM |
| Al16Co16Cr16Fe36Ni16 | 12.81 | -9.8048 | 5.37 | 0.444 | SS+IM |
| Al10(HfNbTiZr)90 | 13.08 | -11.79 | 4.95 | 0.533 | SS+IM |
| Fe36Co21Cr18Ni15Al10 | 12.63 | -7.5744 | 4.43 | 0.644 | SS+IM |
| ZrHfTiCuNi | 13.38 | -26.8 | 10.34 | 0.125 | AM |
| TiZrHfBeNi | 13.38 | -38.45 | 13.56 | 0.073 | AM |
| TiZrCuNbNi | 13.38 | -20.86 | 9.26 | 0.156 | AM |
| TiZrCuNiBe | 13.38 | -30.45 | 12.65 | 0.084 | AM |
| TiZrHfBeCu | 13.38 | -25.63 | 13.18 | 0.077 | AM |
| TiZrHfBeCuNi | 16.06 | -34.65 | 21.78 | 0.034 | AM |
| Ti18.75Zr18.75Cu18.75Nb18.75Ni25 | 13.32 | -23.34 | 9.46 | 0.149 | AM |
| Ti21.25Zr21.25Cu21.25Nb21.25Ni15 | 13.31 | -17.8 | 8.99 | 0.165 | AM |
| Ti21.875Zr21.875Cu21.875Nb21.875Ni12.5 | 13.22 | -16.1 | 8.84 | 0.169 | AM |
| GdTbDyCoAl | 13.38 | -37.27 | 13.60 | 0.072 | AM |
| GdTbDyNiAl | 13.38 | -42.23 | 13.59 | 0.072 | AM |
| GdTbDyFeAl | 13.88 | -26.58 | 13.38 | 0.078 | AM |
| HoErCoAlGd | 13.38 | -37.14 | 13.31 | 0.076 | AM |
| HoErCoAlDy | 13.38 | -37.45 | 12.92 | 0.080 | AM |
| HoErCoAlTm | 13.38 | -37.58 | 12.75 | 0.082 | AM |
| PdPtCuNiP | 13.38 | -32.16 | 8.09 | 0.204 | AM |
| (FeCoNi)75B17.5Si7.5 | 12.8 | -25.08 | 14.62 | 0.060 | AM |
| (FeCoNi)75B15Si10 | 12.92 | -24.91 | 13.61 | 0.070 | AM |
| SrCaYbMgZn | 13.38 | -10.94 | 15.57 | 0.055 | AM |
| (SrCaYbMg)80Zn10Cu10 | 14.53 | -8.13 | 16.48 | 0.053 | AM |
| (ZnSrCaYb)80Li11Mg9 | 14.53 | -9.48 | 15.74 | 0.059 | AM |
| (TiZrHfBe)80Cu17.5Ni2.5 | 14.01 | -25.79 | 13.22 | 0.080 | AM |
| (TiZrHfBe)80Cu15Ni5 | 14.32 | -25.96 | 13.27 | 0.081 | AM |
| (TiZrHfBe)80Cu12.5Ni7.5 | 14.48 | -26.17 | 13.32 | 0.082 | AM |
| (TiZrHfBe)80Cu10Ni10 | 14.53 | -26.4 | 13.37 | 0.081 | AM |
| (TiZrHfBe)80Cu7.5Ni12.5 | 14.48 | -26.65 | 13.41 | 0.081 | AM |
| (TiZrHfBe)80Cu5Ni15 | 14.32 | -26.92 | 13.46 | 0.079 | AM |
| (TiZrHfBe)80Cu2.5Ni17.5 | 14.01 | -27.22 | 13.51 | 0.077 | AM |
| TiZrHfAlAg | 13.38 | -24.32 | 4.90 | 0.557 | AM |
| TiZrHfAlCu | 13.38 | -26.08 | 7.96 | 0.211 | AM |
| TiZrHfAlNi | 13.38 | -41.76 | 8.68 | 0.178 | AM |
| TiZrHfAgCu | 13.38 | -13.12 | 7.90 | 0.214 | AM |
| TiZrHfAgNi | 13.38 | -23.36 | 8.63 | 0.180 | AM |
| TiZrHfCuNi | 13.38 | -27.36 | 10.34 | 0.125 | AM |
| TiZrHfAlAgCu | 14.9 | -22.22 | 7.35 | 0.276 | AM |
| TiZrHfAlAgNI | 14.9 | -31.67 | 7.98 | 0.234 | AM |
| TiZrHfAlCuNi | 14.9 | -34.11 | 9.45 | 0.167 | AM |
| TiZrHfAgCuNi | 14.9 | -21 | 9.44 | 0.167 | AM |
| TiZrHfFeAl | 13.38 | -29.92 | 8.44 | 0.188 | AM |
| TiZrHfFeAg | 13.38 | -11.2 | 8.39 | 0.190 | AM |
| TiZrHfFeCu | 13.38 | -15.84 | 10.15 | 0.130 | AM |
| TiZrHfFeNi | 13.38 | -30.56 | 10.68 | 0.117 | AM |
| TiZrHfCrAg | 13.38 | -5.76 | 7.67 | 0.227 | AM |
| TiZrHfVAl | 13.38 | -21.92 | 6.42 | 0.325 | AM |
| TiZrHfVAg | 13.38 | -4.16 | 6.33 | 0.334 | AM |
| TiZrHfVCu | 13.38 | -8.32 | 8.73 | 0.176 | AM |
| TiZrHfVNi | 13.38 | -24.32 | 9.36 | 0.153 | AM |
| TiZrHfNbNi | 13.38 | -23.36 | 8.54 | 0.183 | AM |
| TiZrHfFeAlAg | 14.9 | -22 | 7.77 | 0.247 | AM |
| TiZrHfFeAlCu | 14.9 | -24.88 | 9.28 | 0.173 | AM |
| TiZrHfCrAgCu | 14.9 | -7.88 | 8.79 | 0.193 | AM |

**Table S5:** Value of optimized parameters for ternary classification in HEA dataset

|  |  |  |
| --- | --- | --- |
| **KNN** | | |
| **Name of the parameter** | **Search range** | **Optimum value** |
| k | [1,20] | 5 |
| Distance function | Euclidean, Manhattan, Minkowski | Minkowski |
| Power | [3, 25] | 2 |
| **ANN** | | |
| **Name of the parameter** | **Search range** | **Optimum value** |
| Hidden layer size | One layer: 5, 10, 20, 30, 40, 50  Two layers: (5, 5), (10,10), (20,20), (30,30), (40,40), (50,50) | (30,30) |
| Activation function | Identity, logistic, tanh, ReLu | ReLu |
| Solver | adam, sgd, lbfgs | adam |
| Initial learning rate | 0.01,0.05,0.1,0.15,0.2 | 0.01 |
| **RF** | | |
| **Name of the parameter** | **Search range** | **Optimum value** |
| number of trees in the forest | 5,10,20,30,40,50,60,70 | 60 |
| minimum sample split | 2, 3, 4, 5, 6 ,7 | 6 |
| maximum depth | 1, 2, 3, 4, 5, 6, 7, 8, 9, 10 | 9 |
| maximum leaf node | [1, 24] | 18 |

**Table S6:** Value of optimized parameters for B1 and B2 binary classification

|  |  |  |  |
| --- | --- | --- | --- |
| **B1 (SS, SS+IM)** | | **B2 (SSS, MSS)** | |
| **KNN** | **ANN** | **KNN** | **ANN** |
| Number of nearest neighbor (k): 5 | Hidden layer size: (10,10) | Number of nearest neighbor (k): 4 | Hidden layer size :(20,20) |
| Distance function: Euclidian | Activation function: ReLU | Distance function: Minkowski, Exponent:3 | Activation function: ReLU |
| Weight: Uniform | Solver: Adam | Weight: distance | Solver: sgd |
| Macro F1 score: 82% | Macro F1 score: 82.5% | Macro F1 score: 59.2% | Macro F1 score: 57.54% |

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