To calculate the parameters in Table S1 for each alloying compositions, we used linear mixture role:

ai and xi are atomic fraction and elemental properties, respectively.

Following equation is used for average atomic volume:

In which R is elemental radius.

Using following equation, the mixing enthalpy is obtained:

In which i , j are considered constituents in the alloying compositions.

Normalized mixing entropy is calculated by the following equation:

R is constant. Gibbs free energy of mixing is calculated from the following equation:

The viscosity, as the kinetic parameter, was calculated as follows:

In which h is Plank constant and NA defines Avogrado number. is molar volume (atomic weight (AW)/density (D)).

(

Mi and ηi are the atomic weight and viscosity of elements.

In which CA is constant.

Table S1: parameters for training the CBNN model

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Elemental properties |  |  |  | Thermo and kinetics |
| Atomic number (AN) | Density (D) | Atomic weight (AW) | Melting point (Tm) | Mixing enthalpy |
| Group (Gp) | Period (P) | Metallic radius (Rm) | Boiling point (Tb) | normalized mixing entropy |
| Covalent radius (Rc) | Heat capacity (Cp) | Thermal conductivity (K) | Electron afﬁnity (Eea) | Gibbs free energy of mixing |
| Heat of fusion (Hf) | Work function (W) | Valence electrons (VEC) | Lattice volume (LP) | Viscosity |
| Mulliken electronegativity (XM) | Pauling electronegativity (XP) | First ionization potential (I1) | Second ionization potential (I2) | Average atomic volume |

Table S2: statistical description of the data space

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Elemental properties | Minimum | Maximum | Average | Standard Deviation |
| Atomic Number | 8.165 | 74.421 | 26.78810746 | 9.326251604 |
| Density | 1.6 | 17.0878 | 6.340959736 | 2.121744338 |
| Valence electron | 2 | 11.22 | 6.048670035 | 1.974780304 |
| Muliken Electronegativity | 0.97205 | 2.23598 | 1.645493489 | 0.14976955 |
| Hmix | -81.12 | 28 | -20.92168214 | 12.57300078 |
| Atomic weight | 17.475875 | 185.26772 | 59.50863042 | 23.34329916 |
| Melting Temperature | 701.722856 | 3460.97 | 1617.863761 | 420.2021466 |
| Heat Capacity | 13.360745 | 34.127 | 24.23054075 | 1.511704607 |
| Pauling Electronegativity | 0.9319 | 2.4131 | 1.702026217 | 0.218309036 |
| Smix | 0 | 1.777764782 | 0.764058909 | 0.254843898 |
| Group | 2 | 13.13 | 8.525810784 | 2.572710446 |
| Boiling Temperature | 1280.8 | 5606.69 | 3212.585205 | 622.394909 |
| Thermal conductivity | 9.308 | 414.44 | 126.3566319 | 72.45514589 |
| First ionization potential | 4.30991 | 9.172851 | 7.292143854 | 0.742035622 |
| Gmix | -3982.014897 | 0 | -1279.753285 | 561.8902703 |
| Period | 2.31 | 6 | 3.92648057 | 0.576748515 |
| Lattice Volume | 10.793 | 292.7764 | 45.54433677 | 41.45436518 |
| Heat of fusion | 6.659 | 53.741 | 17.3624511 | 7.191468168 |
| Second ionization potential | 9.17561875 | 23.5057304 | 17.03180627 | 1.736126496 |
| Viscosity | 1.57E-07 | 2.56E-05 | 1.05E-05 | 3.26E-06 |
| Covalent radius | 0.09162 | 0.20861 | 0.136884437 | 0.016612382 |
| Metallic radius | 0.0892605 | 0.204794 | 0.136465883 | 0.015988785 |
| Average atomic volume | 0.003571394 | 0.038776627 | 0.012039462 | 0.004939945 |
| Electron afﬁnity | -0.49 | 2.083316 | 0.5286451 | 0.326212487 |
| Work Function | 2.6015 | 5.3 | 4.402545681 | 0.390843794 |

Table S3: heat of mixing (KJ/mol) for the studied bonds

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | Zr | Co | Al | W | Si | Ni |
| Zr | 0 | -41 | -44 | -9 | -84 | -49 |
| Co | -41 | 0 | -19 | -1 | -38 | 0 |
| Al | -44 | -19 | 0 | -2 | -19 | -22 |