## Supplementary Information

**Machine learning assisted composition effective design for precipitation strengthened copper alloys**

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### 1 Element features and alloy factors

Table S1 is the collected 79 physical and chemical features of elements. Table S2 is the calculation method of 12 other alloy factors except for the 158 alloy factors. These alloy factors include the elements in the alloy. Type, stoichiometric properties, valence electron orbit occupation properties and solubility of alloying elements.

Table S1. 79 element features

|  |  |
| --- | --- |
| Feature | Source |
| A2 Periodic number start counting left bottom, left-right sequence | [S1] |
| A3 Periodic number start counting top right, right-left sequence |  |
| A4 Periodic number start counting bottom right, right-left sequence |  |
| A5 quantum number |  |
| A6 atomic weight |  |
| A7 mass attenuation coefficient for MoKalpha |  |
| A8 mass attenuation coefficient CrKalpha |  |
| A9 mass attenuation coefficient for CuKalpha |  |
| A10 mass attenuation coefficient FeKalpha |  |
| A11 atomic electron scattering factor at 0.5 |  |
| E1 electronegativity (Martynov&Batsanov) |  |
| E2 electronegativity (Pauling) |  |
| E3 electronegativity (Alfred-Rochow) |  |
| E4 electronegativity absolute |  |
| E5 energy ionization first |  |
| E6 energy ionization second |  |
| E7 energy ionization third |  |
| E8 chemical potential Miedema |  |
| E9 work function |  |
| E10 nWS1/3 Miedema |  |
| E11 nuclear charge effective Slater |  |
| E12 charge nuclear effective (Clementi) |  |
| E13 Electron affinity |  |
| G1 group number |  |
| G2 valence electron number |  |
| G3 valence electron number of s |  |
| G4 valence electron number of p |  |
| G5 valence electron number of d |  |
| G7 unfilled valence electron number |  |
| G8 unfilled valence electron number of s |  |
| G9 unfilled valence electron number of p |  |
| G10 unfilled valence electron number of d |  |
| C1 temperature melting |  |
| C2 temperature boiling |  |
| C3 enthalpy vaporization |  |
| C4 enthalpy melting |  |
| C5 enthalpy atomization |  |
| C6 enthalpy surface Miedema |  |
| C7 enthalpy vacancies Miedema |  |
| C8 energy cohesive Brewer |  |
| C9 modulus compression |  |
| C10 modulus bulk |  |
| C11 modulus rigidity |  |
| C12 modulus Young |  |
| M1 Mendeleev Number t-d start left |  |
| M2 Mendeleev Number t-d start right |  |
| M3 Mendeleev Number d-t start left |  |
| M4 Mendeleev Number d-t start right |  |
| M5 Mendeleev Pettifor |  |
| M6 Mendeleev Pettifor regular |  |
| M7 Mendeleev chemists sequence |  |
| M8 Mendeleev t-d start left |  |
| M9 Mendeleev t-d start right |  |
| M10 Mendeleev d-t start left |  |
| M11 Mendeleev d-t start right |  |
| M12 Mendeleev H,Li,Na,Be,Mg as block t-d start left |  |
| M13 Mendeleev H,Be,Mg t-d start left |  |
| M14 Mendeleev H,Li,Na,Be,Mg t-d start left |  |
| S1 radii pseudo-potential (Zunger) |  |
| S2 radii ionic (Yagoda) |  |
| S3 radii covalent |  |
| S4 radii metal (Waber) |  |
| S5 distance valence electron (Schubert) |  |
| S6 distance core electron (Schubert) |  |
| S7 volume atom (Villars, Daams) |  |
| S8 V2/3 Miedema |  |
| S9 atomic environment number (Villars, Daams) |  |
| S10 Lattice Constants a |  |
| S11 Lattice Constants b |  |
| S12 Lattice Constants c |  |
| S13 radii atomic (coordination number 12) (pm) |  |
| I1 BCC crystal fermi level (eV) | [S2] |
| I2 BCC crystal magnetic moment (μB/atom) |  |
| I3 ground state band gap energy at 0 K (eV/atom) |  |
| I4 ground state energy at 0 K (eV/atom) |  |
| I5 ground state magnetic moment at 0 K (μB/atom) |  |
| I6 ground state volume at 0 K (Å/atom) |  |
| I7 ground state structure space group at 0 K |  |
| I8 density at STP (g/L) |  |

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[S2] Wu, H. et al. Robust FCC solute diffusion predictions from ab-initio machine learning methods. *Comput. Mater. Sci.* **134**,160-165 (2017).

Table S2. 12 other alloy factors

|  |  |  |
| --- | --- | --- |
| Alloy factor | Description | Source |
| O1 number of element | Number of elements | — |
| O2 Stoichiometric attributes P=2 | , is alloy factors, is the content of *i*th element. | [S3] |
| O3 Stoichiometric attributes P=3 |
| O4 Stoichiometric attributes P=5 |
| O5 Stoichiometric attributes P=7 |
| O6 Stoichiometric attributes P=10 |
| O7 Valance orbital occupation attributes s | , F is alloy factor, is the content of ith element, is the number of n-orbital valence electrons of the *i*th element， is the total number of valence electrons of the *i*th element. | [S3] |
| O8 Valance orbital occupation attributes p |
| O9 Valance orbital occupation attributes d |
|  |
| O11 Limit solubility (at.%) | Limit solubility of equilibrium phase diagram | [S4] |
| O12 Room solubility(at.%) | Solubility at room temperature |
| O13 Solubility difference(at.%) | Limit solubility- Solubility at room temperature |

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### 2 Alloy factor screening with 4 algorithms

We used Support Vector Machine (SVM), Bootstrap Aggregating (Bagging), Random Forest (RF) and Gaussian Process Regression (GPR) four algorithms to screen alloy factors, as shown in Figure S1. The number of remaining alloy factors after correlation screening is between 50 and 60. Because different algorithms have different judgments on the importance of alloy factors, the number of remaining alloy factors after screening is different, as shown in Figure S1(a) and (b).



(a)

(b)



(c)

(d)

Figure S1. Alloy factor screening with different algorithm: (a) and (b) are correlation screening recursive elimination, (c) and (d) exhaustive screening.

After recursive elimination of alloy factors that affect hardness, when the remaining alloy factors are 22, 13, 20, and 20, the model errors based on the algorithms SVM, Bagging, RF, and GPR reach the lowest values. After recursive elimination of alloy factors that affect electrical conductivity, when the remaining alloy factors are 17, 14, 16, and 12, the model errors based on the algorithms SVM, Bagging, RF and GPR reach the lowest values respectively.

Figure S1 (c) and (d) are the exhaustive screening results. As the number of alloy factors increases, the model error shows a significant decrease. When the model error is reduced to a minimum, continue to increase the number of alloy factors, and the model error does began to rise. Comparing the alloy factor screening results of different algorithms, when the algorithm is SVM and the number of alloy factors is 5, the hardness model error is the lowest, so SVM is a suitable modeling algorithm for the hardness model, and the key alloy factors affecting hardness are 5. When the algorithm is SVM, the number of alloy factors is 6, the electrical conductivity model has the lowest error, so SVM is a suitable modeling algorithm for the electrical conductivity, and the number of key alloy factors affecting electrical conductivity is 6. It is worth noting that when the machine learning model is established with all alloy factors before screening, the RF algorithm modeling error is the lowest, and after the alloy factor screening, the SVM algorithm modeling error is the lowest, indicating that the appropriate machine learning algorithm is selected.

### 3 Alloy properties after aging treatment

Figure S2 - S5 show the properties of alloys designed iteratively by Bayesian optimization after aging treatment.



(a)

(b)



(c)

Figure S2. Properties of 1st iteration alloys after aging treatment: (a) 1a, (b) 1b, (c) 1c



(c)

(a)

(b)

Figure S3. Properties of 2nd iteration alloys after aging treatment: (a) 2a, (b) 2b, (c) 2c



(b)

(a)



(c)

Figure S4. Properties of 3rd iteration alloys after aging treatment: (a) 3a, (b) 3b, (c) 3c



(b)

(a)



(c)

Figure S5. Properties of 4rd iteration alloys after aging treatment: (a) 4a, (b) 4b, (c) 4c

### 4 Alloy properties after deformation and aging treatment

Figure S6 shows the Cu-1.3Ni-1.4Co-0.56Si-0.03Mg alloy properties after deformation and aging treatment.



(b)

(a)



(d)

(c)

Figure S6. Alloy properties after 1st step and 2nd step aging treatment:   
(a) (b) 1st step aging, (c) (d) 2nd step aging

5 Alloy composition and properties

Table S3. The composition and properties of the alloy designed in this paper and those reported in the literature

|  |  |  |  |
| --- | --- | --- | --- |
| Alloy (wt%) | UTS (MPa) | EC (%IACS) | Source |
| Cu-1.3Ni-1.4Co-0.56Si-0.03Mg | 858 | 47.6 | This study |
| Cu-2Ni-0.5Si-0.1Mg | 630 | 44 | [S5] |
| Cu-1.82Ni-1.62Co-0.86Si | 706.8 | 43.8 | [S6] |
| Cu-2.51Ni-0.51Si-0.37Co | 757 | 44 | [S7] |
| Cu-2.51Ni-0.51Si-0.37Cr | 834 | 44.8 | [S7] |
| Cu-1.8Ni-1.04Si-1.02Co-0.2Zr | 645 | 45 | [S8] |
| Cu-2.11Ni-0.53Si-0.18Zr | 667 | 40 | [S9] |
| Cu-6.02Ni-1.38Si-0.13Ti | 939 | 42 | [S10] |
| Cu-4.38Ni-1Si-0.09Ti | 737 | 43 | [S11] |
| Cu-4.38Ni-0.94Si-0.18Ti | 791 | 40.3 | [S11] |
| Cu-3Ni-0.52Si-0.15P | 850 | 45 | [S12] |
| Cu-2Ni-0.5Si-0.15Zr | 587 | 47.5 | [S13] |
| Cu-2Ni-0.5Si-0.15Cr-0.15Zr | 706 | 48.2 | [S13] |
| Cu-3Ni-0.5Si-0.2Cr | 806 | 46 | [S14] |

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