Supplementary Materials

Rapid design of high-strength high-conductivity copper alloys via machine learning and NSGA-II multi-objective optimization

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1. Machine learning and NSGA-II hyperparameters

Supplementary Table 1. The actual compositions by ICP

Element	Cu	Ni	Co	Si	Mg	Ag
ICP (wt%)	Bal	0.63	1.60	0.46	0.05	0.41

Supplementary Table 2. Seven key alloy descriptors formulas

Factors	Formula	Description
delta_r	$delta_r = \sqrt{\sum_{i=1}^{n} C_i * \left(1 - \frac{r_i}{r}\right)^2}$	Atomic radius difference
delta_chi	$delta_{chi} = \sqrt{\sum_{i=1}^{n} C_i * (\chi - \chi_i)^2}$	electronegativity difference
VEC	$VEC = \sum_{i=1}^{n} C_i * VEC_i$	Valence electron concentration
Gpa	$Gpa = \sum_{i=1}^{n} C_i * G_i$	Shear modulus difference
sigma2	$sigma2 = \frac{\sum_{i=1}^{n} \left[C_i * E_i - \left(\frac{\sum_{i=1}^{n} C_i * E_i}{n}\right)\right]^2}{n}$	Second ionization energy variance
e_a	$e_a = \sum_{i=1}^{n} C_i * (e/\mathrm{a})_i$	Electron ratio
W	$W = \left(\sum_{i=1}^{n} C_i * w_i\right)^6$	The sixth power of the work function

Collection of key parameters in common material areas. variable definitions in the following formulas: C_i is the molar content of each element in the alloy; VEC_i represents the valence electron concentration of each atom; r_i denotes the atomic radius of each element; G_i is the shear modulus of each element; w_i refers to the work function of each atom; E_i is the second ionization energy of each element; χ_i indicates the electronegativity of each atom; and R is a constant with a value of 8.314.

Supplementary Table 3. UTS model hyperparameters

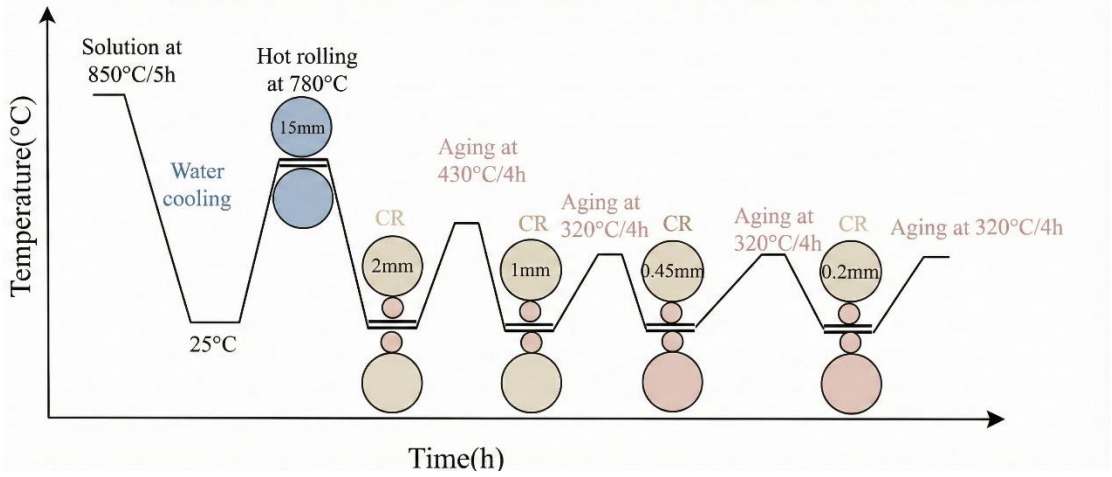
Machine learning	UTS-Optimal hyperparameters
DT	max_depth=9;min_samples_spilt=5;min_samples_leaf=1
SVM	C=1500;epsilon=1;kernel=rbf;gamma=0.01
RF	n_estimators=300;max_depth=None;min_samples_spilt=2
XGBoost	n_estimators=300;max_depth=5;learing_rate=0.1
GBR	n_estimators=250;max_depth=3;learing_rate=0.1

Supplementary Table 4. EC model hyperparameters

Machine learning	EC-Optimal hyperparameters
DT	max_depth=9;min_samples_spilt=10;min_samples_leaf=4
SVM	C=500;epsilon=1;kernel=rbf;gamma=auto
RF	n_estimators=300;max_depth=None;min_samples_spilt=2
XGBoost	n_estimators=300;max_depth=5;learing_rate=0.1
GBR	n_estimators=200;max_depth=5;learing_rate=0.1

Supplementary Table 5. Stacking- hyperparameters

Base-model	parameter	value
RF	n_estimators	200
GBR	n_estimators	200
SVR	kernel	rbf
Linear Regressor	default	default



Supplementary Figure 1. Actual process flow diagram.

Machine Learning Evaluation Metrics:

$$R^2 = 1 - \frac{\sum (y_i - \hat{y}_i)^2}{\sum (y_i - \bar{y}_i)^2}$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}$$

$$MAE = \frac{1}{n}\sum_{i=1}^{n} |y_i - \hat{y}_i|$$

Combination-A: alloying factors+ process parameters

Combination-B: element content + process parameters

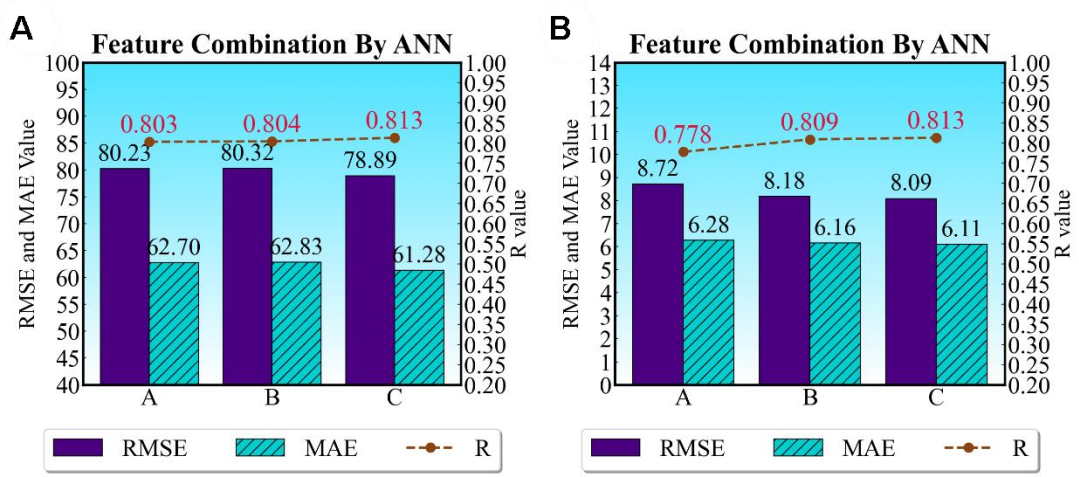
Combination-C: element content + alloying factors+ process parameters

Supplementary Table 6. UTS-Combination

Feature Combination	R^2	RMSE	MAE
A	0.803	80.23	62.7
B	0.804	80.32	62.83
C	0.813	78.89	61.28

Supplementary Table 7. EC-Combination

Feature Combination	R^2	RMSE	MAE
A	0.778	8.72	6.28
B	0.809	8.18	6.16
C	0.813	8.09	6.11



Supplementary Figure 2. Feature combination result by Ann.

Supplementary Table 8. Process parameters fixed for the pareto set

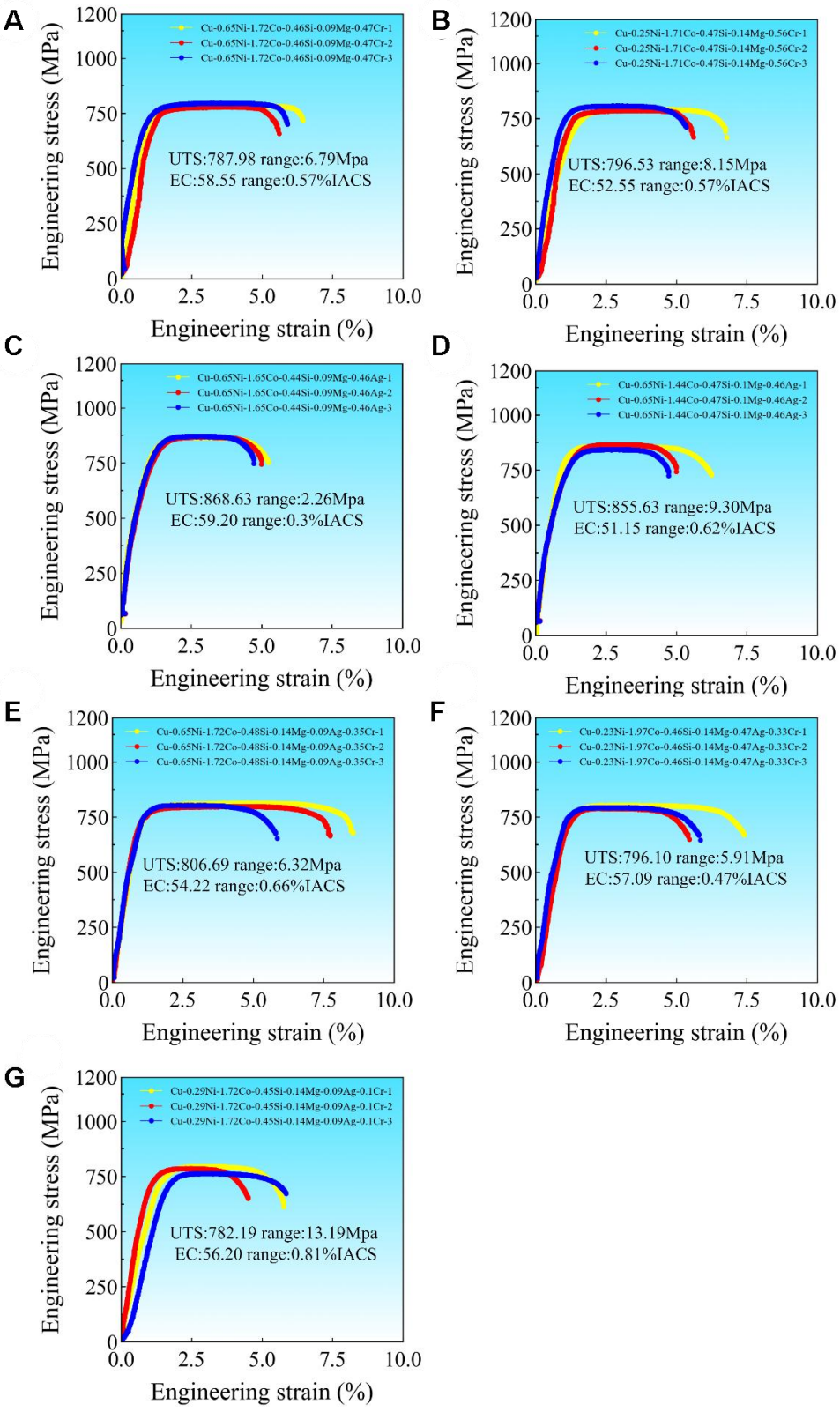
Process parameter	Value
Solid solution temperature	850C°
Solid solution time	5h
Hot rolling temperature	780C°
Hot rolled deformation	50%
Aging temperature_1	430C°
Aging time_1	4h
Clod rolling temperature	25C°
Clod rolled deformation	98%
Aging temperature_2	320C°
Aging time_2	4h

Supplementary Table 9. NSGA-II algorithm hyperparameters search results

	Pop_size	Crossover_prob	Crossover_eta	Mutation_prob	Mutation_eta
a	72	0.600473876400918	17	0.2293075615795751	10
b	74	0.7640864323427644	9	0.23169161640501973	11
C	109	0.701744278638143	5	0.01	20

(a: Cu-Ni-Co-Si-Mg-Cr; b: Cu-Ni-Co-Si-Mg-Ag; c: Cu-Ni-Co-Si-Mg-Cr-Ag) in order.

2. Tensile stress-strain curve

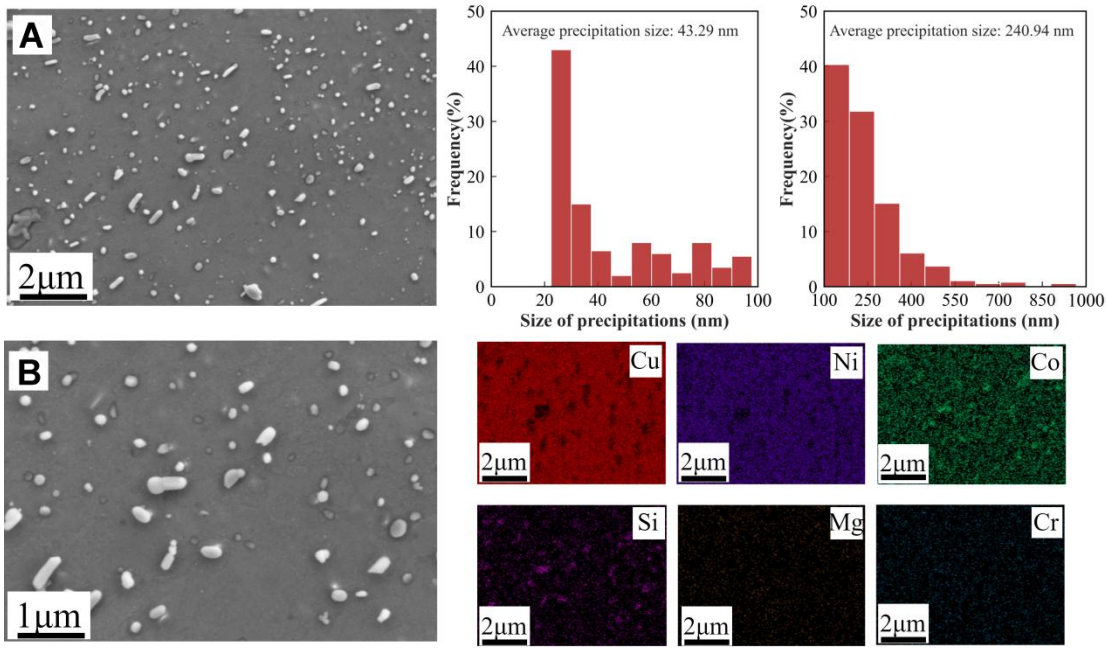


Supplementary Figure 3. Seven alloys stensile stress-strain curve.

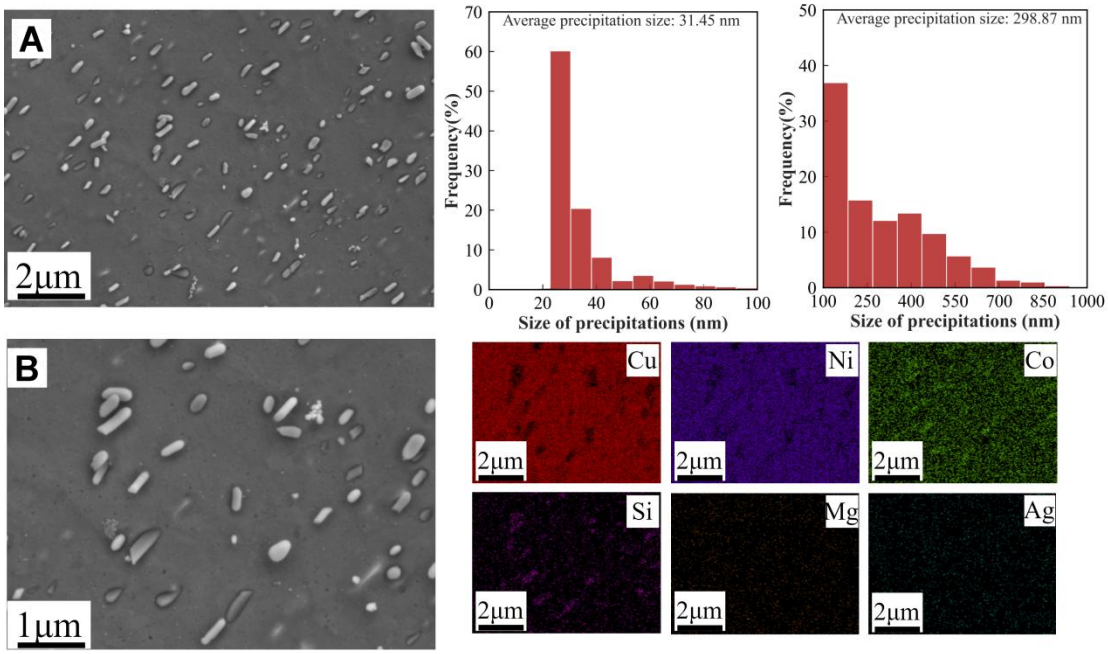
Supplementary Table 10. Prediction error of alloy strength and electrical conductivity

Alloy id	UTS inaccuracy (%)	EC inaccuracy (%)
1	-10.66	7.72
2	-9.28	-5.85
3	-0.29	-0.24
4	-0.59	-17.18
5	-7.87	-11.79
6	-8.39	-8.57
7	-12.41	-3.52
Average	-7.07	-7.84

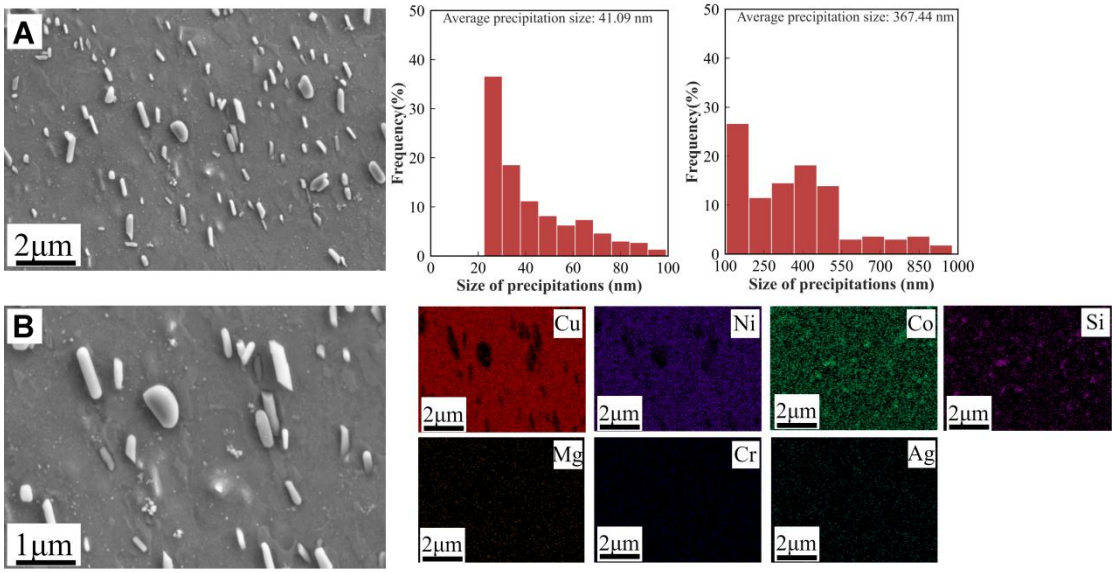
3. SEM-Precipitation phase distribution



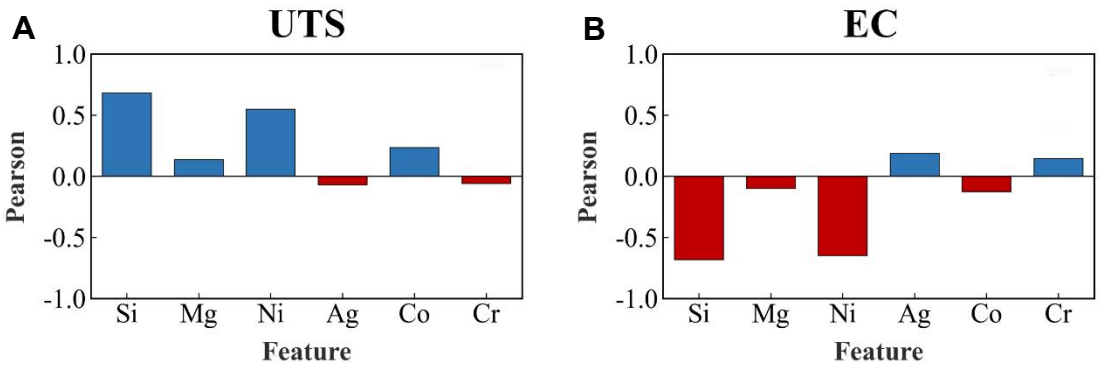
Supplementary Figure 4. SEM and EDS results of 2-alloy.



Supplementary Figure 5. SEM and EDS results of 3-alloy.



Supplementary Figure 6. SEM and EDS results of 5-alloy.



Supplementary Figure 7. Correlation coefficients between elements and properties.