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An Effective Framework for Predicting Performance of Solid-Solution Copper Alloys Using a Feature Engineering Technique in Machine Learning

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Table S1. The original data of SSCAs used in this work [#].

Cu	Mg	Sn	Zn	Al	Thickness	Reduction Ratio	Heat-Treat		HV	EC
							Temperature	Time		
100	0	0	0	0	2	75%	25	60	126.88	99.21
99.3	0.7	0	0	0	2	75%	25	60	141.53	79.59
98	2	0	0	0	2	75%	25	60	182.94	56.16
97	3	0	0	0	2	75%	25	60	186.12	47.57
96	4	0	0	0	2	75%	25	60	200.16	40.46
95	5	0	0	0	2	75%	25	60	221.23	35.35
94	6	0	0	0	2	75%	25	60	239	34.48
99.6	0	0.4	0	0	2	75%	25	60	144.14	58.11
99	0	1	0	0	2	75%	25	60	167.62	37.07
98	0	2	0	0	2	75%	25	60	203.59	22.01
97	0	3	0	0	2	75%	25	60	228.55	15.86
94.4	0	5.6	0	0	2	75%	25	60	271.96	10.52
92	0	0	8	0	2	75%	25	60	149.2	47.04
87	0	0	13	0	2	75%	25	60	176.54	36.11
80	0	0	20	0	2	75%	25	60	202.4	28.32
70	0	0	30	0	2	75%	25	60	209.46	23.49
96	0	0	0	4	2	75%	25	60	148.9	29.2
92	0	0	0	8	2	75%	25	60	207.45	18.23
88	0	0	0	12	2	75%	25	60	241.93	14.44
85	0	0	0	15	2	75%	25	60	251.88	12.85
82	3	0	0	15	2	75%	25	60	288.24	11.97
100	0	0	0	0	2	75%	50	60	126.1	99.28
100	0	0	0	0	2	75%	100	60	131	99.4
100	0	0	0	0	2	75%	150	60	125.66	100.91
100	0	0	0	0	2	75%	200	60	74.12	101.02
100	0	0	0	0	2	75%	250	60	68.02	101.14
100	0	0	0	0	2	75%	300	60	67.99	102.71
100	0	0	0	0	2	75%	350	60	69.85	104.32
100	0	0	0	0	2	75%	400	60	67.17	104.45
100	0	0	0	0	2	75%	450	60	61.08	101.62
100	0	0	0	0	2	75%	500	60	65.22	103.2

100	0	0	0	0	2	75%	550	60	65.56	103.32
100	0	0	0	0	2	75%	600	60	64.77	104.96
98	2	0	0	0	2	75%	50	60	183.68	56.87
98	2	0	0	0	2	75%	100	60	187.82	57.36
98	2	0	0	0	2	75%	150	60	185.13	57.86
98	2	0	0	0	2	75%	200	60	185.86	57.9
98	2	0	0	0	2	75%	250	60	177.12	58.89
98	2	0	0	0	2	75%	300	60	169.89	60.42
98	2	0	0	0	2	75%	350	60	164.93	58.97
98	2	0	0	0	2	75%	400	60	95.96	59.5
98	2	0	0	0	2	75%	450	60	91	60.54
98	2	0	0	0	2	75%	500	60	89.84	60.59
98	2	0	0	0	2	75%	550	60	79.58	61.14
98	2	0	0	0	2	75%	600	60	73.86	61.19
94	6	0	0	0	2	75%	50	60	240.88	33.85
94	6	0	0	0	2	75%	100	60	243.12	34.02
94	6	0	0	0	2	75%	150	60	244.22	34.03
94	6	0	0	0	2	75%	200	60	238.89	34.21
94	6	0	0	0	2	75%	250	60	233.93	35.06
94	6	0	0	0	2	75%	300	60	222.92	36.49
94	6	0	0	0	2	75%	350	60	219.1	38.67
94	6	0	0	0	2	75%	400	60	198.23	42.84
94	6	0	0	0	2	75%	450	60	174.72	48.66
94	6	0	0	0	2	75%	500	60	142.11	45.89
94	6	0	0	0	2	75%	550	60	134.5	43.42
94	6	0	0	0	2	75%	600	60	106.06	38.76
70	0	0	30	0	2	75%	50	60	210.2	23.31
70	0	0	30	0	2	75%	100	60	207.89	23.47
70	0	0	30	0	2	75%	150	60	221.88	23.71
70	0	0	30	0	2	75%	200	60	235.86	24.61
70	0	0	30	0	2	75%	250	60	214.61	24.96
70	0	0	30	0	2	75%	300	60	129.36	26.73
70	0	0	30	0	2	75%	350	60	115.31	26.74
70	0	0	30	0	2	75%	400	60	113.01	26.84
70	0	0	30	0	2	75%	450	60	100.47	26.95
70	0	0	30	0	2	75%	500	60	99.31	26.96
70	0	0	30	0	2	75%	550	60	84.12	27.17
70	0	0	30	0	2	75%	600	60	83.33	27.18
85	0	0	0	15	2	75%	50	60	253	12.97
85	0	0	0	15	2	75%	100	60	254.1	12.97
85	0	0	0	15	2	75%	150	60	257.86	13.04
85	0	0	0	15	2	75%	200	60	273.36	13.51
85	0	0	0	15	2	75%	250	60	280.52	14.23
85	0	0	0	15	2	75%	300	60	197.92	15.07
85	0	0	0	15	2	75%	350	60	178.95	15.17
85	0	0	0	15	2	75%	400	60	178.16	15.27
85	0	0	0	15	2	75%	450	60	166	15.18
85	0	0	0	15	2	75%	500	60	145.52	15.24
85	0	0	0	15	2	75%	550	60	122.76	15.48
85	0	0	0	15	2	75%	600	60	117.8	15.82
82	3	0	0	15	2	75%	50	60	289.74	12.12
82	3	0	0	15	2	75%	100	60	296.53	12.3

82	3	0	0	15	2	75%	150	60	310.51	12.5
82	3	0	0	15	2	75%	200	60	322.22	12.77
82	3	0	0	15	2	75%	250	60	320.3	12.88
82	3	0	0	15	2	75%	300	60	310.42	13.14
82	3	0	0	15	2	75%	350	60	299.4	13.24
82	3	0	0	15	2	75%	400	60	262.25	14.19
82	3	0	0	15	2	75%	450	60	225.47	14.36
82	3	0	0	15	2	75%	500	60	218.25	14.16
82	3	0	0	15	2	75%	550	60	198.52	14.28
82	3	0	0	15	2	75%	600	60	172.35	14.28
94.4	0	5.6	0	0	2	75%	50	60	275.73	10.5
94.4	0	5.6	0	0	2	75%	100	60	277.97	10.58
94.4	0	5.6	0	0	2	75%	150	60	277.18	10.58
94.4	0	5.6	0	0	2	75%	200	60	269.95	10.65
94.4	0	5.6	0	0	2	75%	250	60	263.1	10.76
94.4	0	5.6	0	0	2	75%	300	60	252.08	10.94
94.4	0	5.6	0	0	2	75%	350	60	153.95	10.94
94.4	0	5.6	0	0	2	75%	400	60	139.9	11.05
94.4	0	5.6	0	0	2	75%	450	60	123.96	11.03
94.4	0	5.6	0	0	2	75%	500	60	114.08	10.95
94.4	0	5.6	0	0	2	75%	550	60	104.96	10.95
94.4	0	5.6	0	0	2	75%	600	60	107.2	11.04

Note: Only the first 21 pieces of data (highlighted by yellow color) are used for EC analysis.

Table S2. Comprehensive description of the elements' properties.

No.	Names	Units
P1	ΔH interface M in O (Miedema)	$kJ*mol^{-1}$
P2	ΔH interface M in S (Miedema)	$kJ*mol^{-1}$
P3	ΔH interface O in M (Miedema)	$kJ*mol^{-1}$
P4	ΔH interface S in M	$kJ*mol^{-1}$
P5	γ-free electron to specific heat	$mJ*mol^{-1}*K^{-2}$
P6	Atomic concentration	10^{23} m^{-3}
P7	Atomic electron scattering factor at 0.5	
P8	Atomic environment number (Villars, Daams)	
P9	Atomic number start counting left top, left-right sequence	
P10	Atomic weight	10^{-3} kg
P11	Boiling temperature	K
P12	Bulk modulus	GPa
P13	Charge nuclear effective (Clementi)	
P14	Chemical potential (Miedema)	
P15	Compression modulus	GPa
P16	Conductivity electrical	10^4 $Ohm^{-1}*cm^{-1}$
P17	Conductivity thermal	$J*mol^{-1}*K^{-1}$
P18	Debye temperature	K
P19	Density	$kg*m^{-3}$
P20	Distance from core electron (Schubert)	A
P21	Distance from valence electron (Schubert)	A
P22	Electrochemical weight equivalent	$mg*K^{-1}$
P23	Electron affinity	$kJ*mol^{-1}$
P24	Electronegativity (Allred-Rochow)	

P25	Electronegativity (Martynov&Batsanov)	
P26	Electronegativity (Pauling)	
P27	Electronegativity absolute	
P28	Energy cohesive (Brewer)	$J*mol^{-1}$
P29	Energy of ionization first	$kJ*mol^{-1}$
P30	Energy of ionization second	$kJ*mol^{-1}$
P31	Energy of ionization third	$kJ*mol^{-1}$
P32	Enthalpy of atomization	$kJ*mol^{-1}$
P33	Enthalpy of melting	$kJ*mol^{-1}$
P34	Enthalpy of surface (Miedema)	$kJ*mol^{-1}$
P35	Enthalpy of vacancies (Miedema)	$kJ*mol^{-1}$
P36	Enthalpy of vaporization	$kJ*mol^{-1}$
P37	Entropy of solid	$J*mol^{-1}*K^{-1}$
P38	Group number	
P39	Hardness (Brinell)	MPa
P40	Linear thermal expansion coefficient	$10^{-6}*K^{-1}$
P41	Magnetic frequency of nuclei	
P42	Magnetic resonance	MHz
P43	Magnetic susceptibility	m^3*kg^{-1}
P44	Mass attenuation coefficient CrKα	cm^2*g^{-1}
P45	Mass attenuation coefficient FeKα	cm^2*g^{-1}
P46	Mass attenuation coefficient for CuKα	cm^2*g^{-1}
P47	Mass attenuation coefficient for MoKα	cm^2*g^{-1}
P48	Melting temperature	K
P49	Mendeleev chemists sequence	
P50	Mendeleev d-t start left	
P51	Mendeleev d-t start right	
P52	Mendeleev H d-t start left	
P53	Mendeleev H d-t start right	
P54	Mendeleev H t-d start left	
P55	Mendeleev H t-d start right	
P56	Mendeleev Pettifor	
P57	Mendeleev Pettifor regular	
P58	Mendeleev t-d start left	
P59	Mendeleev t-d start right	
P60	Modulus of rigidity	GPa
P61	Molar heat capacity	$J*mol^{-1}*K^{-1}$
P62	Moment nuclear magnetic	mu
P63	Nuclear charge effective (Slater)	
P64	nW1/3 (Miedema)	$a.u.^{-1/3}$
P65	Oxidation state first	
P66	Periodic number start counting bottom right, right-left sequence	
P67	Periodic number start counting left bottom, left-right sequence	
P68	Periodic number start counting top right, right-left sequence	
P69	Poisson's ratio	
P70	Quantum number	
P71	Radii covalent	pm
P77	Radii metal (Waber)	A
P78	Radii pseudo-potential (Zunger)	a.u.
P79	Resistivity electrical	10^{-8} Ohm*m
P80	Sound velocity	$m*s^{-1}$
P81	Spectral lines no	

P82	Spin nuclei	h
P83	Surface tension at T_m	$mJ*m^{-2}$
P84	Thermal neutron capture cross section	barns
P85	V2/3 (Miedema)	cm^2
P86	Valence electron number	
P87	Vapour pressure at T_m	$N*m^{-2}$
P88	Volume of atom (Villars, Daams)	10^{-2} nm^3
P89	Work function	eV
P90	Young's modulus	GPa

Table S3. Remaining features after each screening step.

Property	Screening Step	Features After Screening
HV	Removing features with low variance	P1_mean, P2_mean, P3_mean, P4_mean, P5_mean, P7_mean, P19_mean, P21_mean, P22_mean, P24_mean, P25_mean, P26_mean, P43_mean, P47_mean, P49_mean, P56_mean, P65_mean, P77_mean, P78_mean, P80_mean, P84_mean, P85_mean, P87_mean, P88_mean, P1_var, P2_var, P3_var, P4_var, P5_var, P7_var, P8_var, P9_var, P10_var, P13_var, P18_var, P19_var, P20_var, P21_var, P22_var, P24_var, P25_var, P26_var, P27_var, P29_var, P30_var, P31_var, P37_var, P38_var, P39_var, P43_var, P47_var, P49_var, P50_var, P51_var, P52_var, P53_var, P54_var, P55_var, P56_var, P57_var, P58_var, P59_var, P60_var, P61_var, P63_var, P64_var, P65_var, P66_var, P67_var, P68_var, P70_var, P77_var, P78_var, P79_var, P80_var, P84_var, P86_var, P87_var, P89_var, HT
	Correlation screening	P88_mean, P8_var, P20_var, P24_var, P26_var, P27_var, P30_var, P37_var, P56_var, P60_var, P64_var, P77_var, P89_var, HT
	Recursive elimination	P26_var, P56_var, P77_var, P24_var, HT
EC	Removing features with low variance	P1_mean, P2_mean, P3_mean, P4_mean, P19_mean, P21_mean, P22_mean, P24_mean, P25_mean, P26_mean, P49_mean, P50_mean, P51_mean, P52_mean, P53_mean, P54_mean, P55_mean, P56_mean, P57_mean, P58_mean, P59_mean, P65_mean, P77_mean, P78_mean, P84_mean, P85_mean, P87_mean, P88_mean, P1_var, P2_var, P3_var, P4_var, P5_var, P6_var, P7_var, P9_var, P10_var, P11_var, P13_var, P14_var, P15_var, P18_var, P19_var, P20_var, P21_var, P22_var, P23_var, P24_var, P25_var, P26_var, P27_var, P28_var, P29_var, P30_var, P31_var, P32_var, P36_var, P37_var, P38_var, P39_var, P41_var, P42_var, P43_var, P47_var, P49_var, P50_var, P51_var, P52_var, P53_var, P54_var, P55_var, P56_var, P57_var, P58_var, P59_var, P60_var, P63_var, P64_var, P65_var, P66_var, P67_var, P68_var, P69_var, P70_var, P77_var, P78_var, P79_var, P80_var, P81_var, P82_var, P84_var, P86_var, P87_var, P89_var
	Correlation screening	P1_mean, P56_mean, P58_mean, P4_var, P6_var, P18_var, P20_var, P24_var, P25_var, P27_var, P30_var, P37_var, P39_var, P41_var, P49_var, P63_var, P64_var, P84_var, P89_var
	Recursive elimination	P39_var, P6_var, P25_var, P18_var

Note: "_mean" denotes the mean value of the property, while "_var" indicates the variance value of the property.