Supplementary Information

Development of an accurate "composition-process-properties" dataset for SLMed Al-Si-(Mg) alloys and its application in alloy design

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Table S1. The statistical results (range, mean, and standard deviation) of the concentration of each element, Ed, rotation angle, tensile direction, UTS, YS, and EL among the 167 data before data cleaning.

	W(Si) (wt%)	W(Mg) (wt%)	Ed (J/mm^3)	Rotation (°)	Direction (°)	UTS (MPa)	YS (MPa)	EL (%)
count	176	176	176	176	176	176	176	176
mean	9.62	0.27	56.62	74.26	25.06	373.56	239.63	7.33
std	2.19	0.22	27.07	12.31	40.45	68.36	56.17	4.61
min	4.07	0.00	13.33	45.00	0.00	185.20	103.00	0.54
25%	7.19	0.00	39.99	67.00	0.00	321.13	206.38	3.91
50%	10.00	0.30	50.79	67.00	0.00	385.00	243.40	6.70
75%	11.87	0.46	62.08	90.00	90.00	426.40	287.20	9.15
max	12.47	0.65	176.19	90.00	90.00	514.00	334.00	22.00

Table S2. The statistical results (range, mean, and standard deviation) of the concentration of each element, Ed, rotation angle, tensile direction, UTS, YS, and EL among the model-constructing data set after data cleaning.

	W(Si) (wt%)	W(Mg) (wt%)	Ed (J/mm^3)	Rotation (°)	Direction (°)	UTS (MPa)	YS (MPa)	EL (%)
count	142	142	142	142	142	142	142	142
mean	9.29	0.31	59.36	72.58	24.72	379.69	237.90	8.36
std	2.19	0.22	27.37	11.88	40.31	67.66	58.34	4.36
min	4.07	0.00	17.92	45.00	0.00	246.00	103	2.40
25%	7.14	0.00	45.55	67.00	0.00	326.43	198.03	5.23
50%	10.00	0.30	52.43	67.00	0.00	390.50	243.40	7.55
75%	10.38	0.55	62.08	90.00	90.00	434.19	290.28	9.88
max	12.47	0.65	176.19	90.00	90.00	514.00	327.00	22.00

Table S3. The optimized hyperparameters of MLPReg model.

Hyperparameter	Value
neurons number	(100,200)
activation function	'ReLU'
solver	'L-BFGS'
alpha	0.6
random state	84
tol	0.0001

The hyperparameters of the MLPReg model were optimized by a random search strategy with a 10% testing data set. The structure of the optimized MLPReg model was 5×2×3 (5 input features, 2 hidden layers, and 3 output features), and the number of neurons in the two hidden layers is 100 and 200, respectively. The rectified linear unit (ReLU) function is used as the activation function. 'L-BFGS' was used as the solver for weight optimization. The best combinations of hyperparameters are the following: 'alpha' = 0.6(strength of the L2 regularization term), 'random state' = 84(determines random number generation for weights and bias initialization), and 'tol' = 0.0001(tolerance for the optimization).

Table S4. The experimental data for model accuracy verification, which are unduplicated with the data set used to establish the model.

ID	Alloy	W(Si) (wt%)	W(Mg) (wt%)	Ed (J/mm^3)	Rotation (°)	Direction (°)	UTS (MPa)	YS (MPa)	EL (%)
A1	Al-12Si	12.00	0	39.60	79	0	418.9	220.5	3.91
A2	Al-12Si	12.00	0	39.60	79	0	369.3	202.2	4.38
A3	Al-12Si	12.00	0	39.99	73	90	302.7	276.6	2.3
B1	AlSi10Mg	10.81	0.56	80.13	67	90	384.6	227.3	7.41
B2	AlSi10Mg	10.00	0.30	38.70	67	0	425	246	9.5
B3	AlSi10Mg	10.00	0.30	38.70	67	90	402	223	5.7
C1	A357	7.00	0.60	94.35	67	0	413	222	11
C2	A357	7.04	0.52	60.61	67	0	427	280	10.5
C3	A357	7.04	0.52	60.61	67	90	395	232	5.1

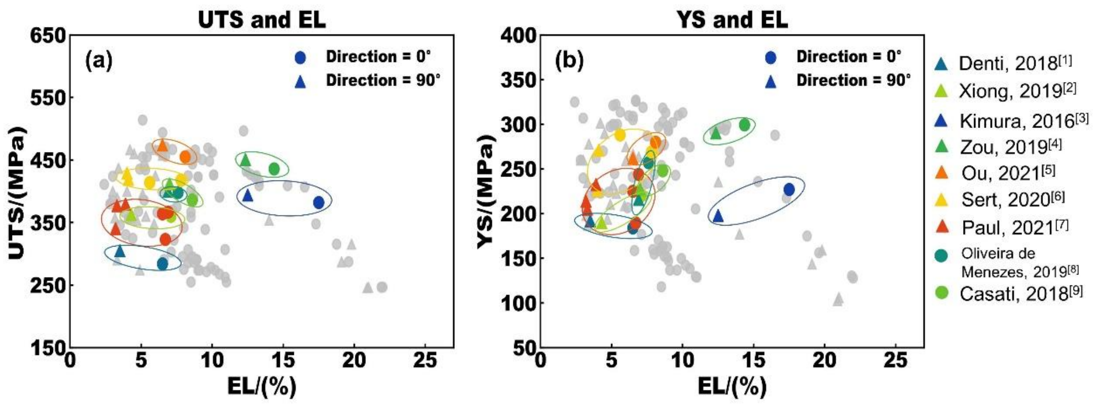

Figure S1. The UTS, YS, and EL for the alloys under 0° and 90° test direction, respectively. Those data points marked by the same color mean that they come from the same report with the same preparation condition[1–9].

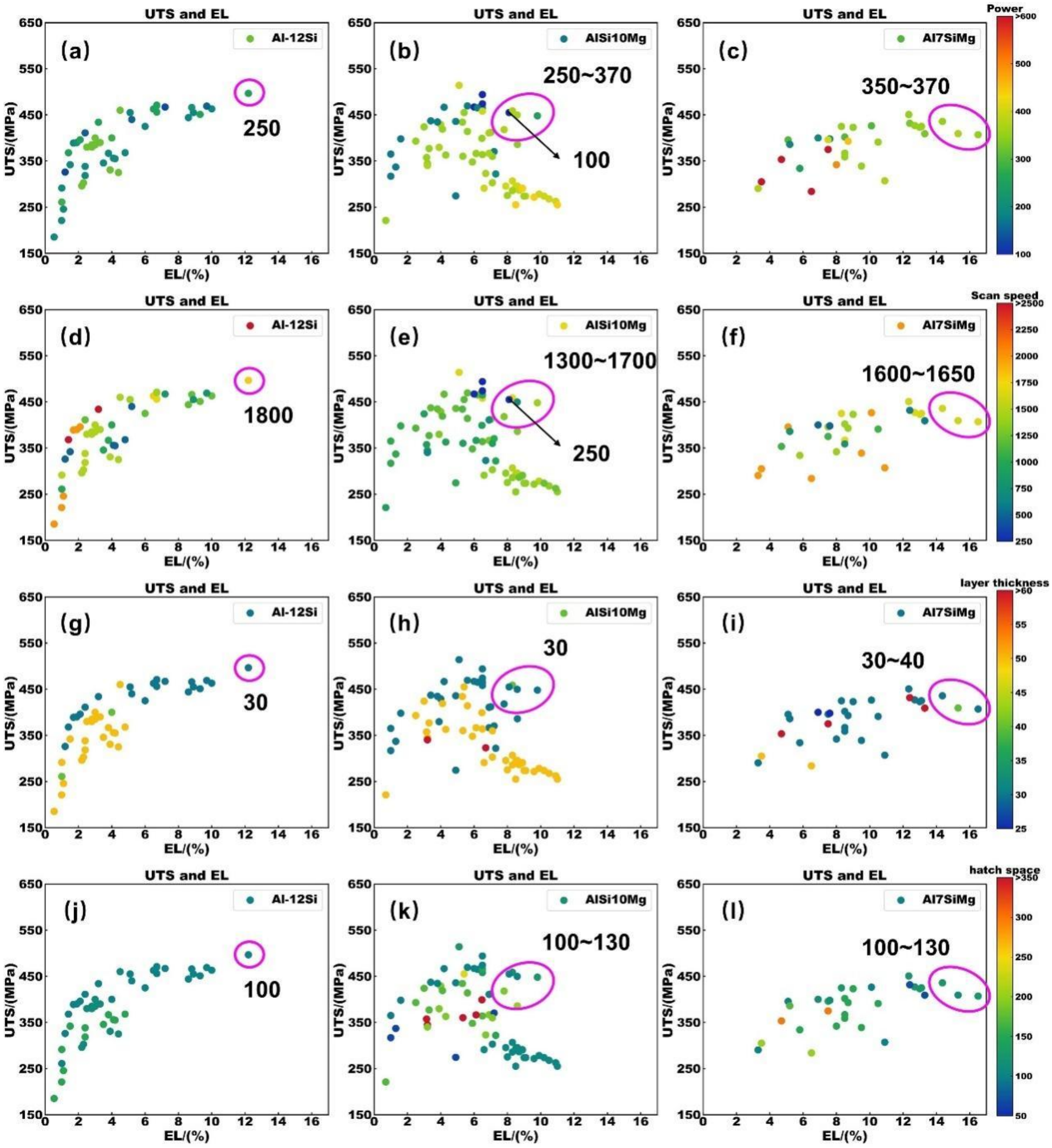

Figure S2. The impact of d laser power, scan speed, hatch space, and layer thickness on the properties of Al12Si (a, d, g, j), AlSi10Mg (b, e, h, k), and Al7SiMg (c, f, i, l).

Data analysis

Based on the existing experimental data set, the effect of detail manufacturing parameters (laser power, scan speed, hatch space, and layer thickness) on the properties of SLMed Al-Si-Mg alloys were further investigated and analyzed. As shown in **Figure S2 a-f**, high strength and high ductility can be achieved when high laser power and slow scan speed are applied in Al12Si and AlSi10Mg preparation. This can be explained by the results of Suzuki's study[10]. When laser power became higher, and scan speed became lower, the energy density and the alloy density increased, the crystal grain size and the fraction of <001> oriented α-Al crystal grains toward the building direction increased, and the high concentration of solute Si in α-Al matrix led to good mechanical property. In addition, as can be seen in **Figure S2 g-l**, the properties of the alloy are usually lower when the layer thickness and the hatch space are larger. According to **Eq. 4**, the Ed reduces with the layer thickness and hatch space increasing. Lower Ed is not conducive to improving the performance of the alloy. As a result, the optimal layer thickness is 30 μm~40 μm, and the optimal hatch space is 100 μm~130 μm. Laser power can vary from 250 W to 370 W; correlatedly, the scan speed varies from 1300 mm/s to 1800 mm/s. The optimum laser power value decreases as the Si content increases, but the optimal scan speed increases as the Si content increases. For Al7SiMg alloy, the optimal combination of laser power and scanning speed is 350 W~370 W with 1600 mm/s ~1650 mm/s, but 250 W with 1800 mm/s to Al12Si alloy. In other words, the variation of Ed mainly depends on laser power and scanning speed.

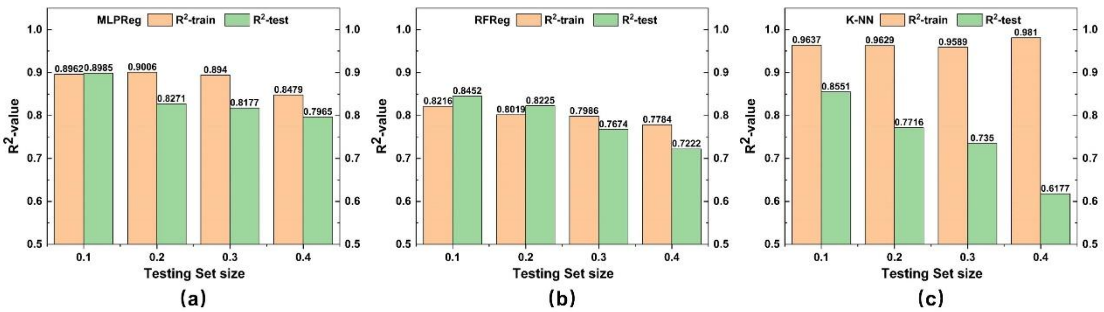

Figure S3. R^2 score of (a) MLPReg, (b) RFReg, and (c) K-NN, with the size of the testing set varying from 10% to 40%.

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