

Supplementary Materials

Machine-learning-enabled composition–process co-design of heat-resistant cast aluminum alloys with superior elevated-temperature strength

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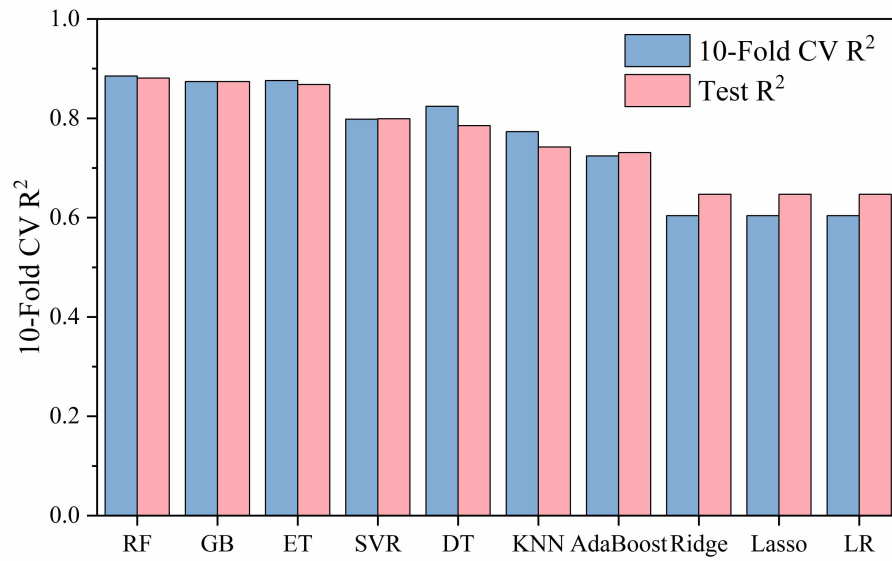
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Note S1. Benchmark comparison of candidate regression models

A systematic benchmark comparison was conducted using ten representative regression algorithms, including Random Forest (RF), Gradient Boosting (GB), Extra Trees (ET), support vector regression (SVR), Decision Tree (DT), K-nearest neighbors (KNN), AdaBoost (AdaBoost), Ridge Regression (Ridge), Lasso Regression (Lasso), and Linear Regression (LR). All models were trained and evaluated using the same selected feature subset, identical training/test partitioning, and the same 10-fold cross-validation strategy to ensure a fair comparison. The model performance was assessed using the coefficient of determination (R^2), root mean square error (RMSE), and mean absolute error (MAE).

As shown in Supplementary Figure 1 and Supplementary Table 1, Random Forest (RF) exhibited the best overall predictive performance among the evaluated candidate models. Specifically, RF achieved the highest mean 10-fold cross-validation (R^2) of 0.885. On the independent test set, RF also yielded the highest (R^2) of 0.881, together with the lowest RMSE of 32.944 MPa and a low MAE of 22.639 MPa. Gradient Boosting (GB) and Extra Trees (ET) also showed competitive predictive accuracy; however, their independent test-set performance was slightly inferior to that of RF. Although ET exhibited the lowest mean cross-validation MAE, its test-set R^2 , RMSE, and MAE were all slightly poorer than those of RF. Therefore, RF was selected as the final predictive model because it provided the best overall balance among prediction accuracy, robustness, and generalization capability.

The generalization capability and robustness of RF were further supported by the consistency between the cross-validation and independent test-set results. The difference between the overall cross-validation (R^2) and the test-set (R^2) was only 0.005, while the corresponding RMSE values were 32.817 MPa and 32.944 MPa, respectively. In addition, the standard deviation of the 10-fold cross-validation (R^2) for RF was 0.023, indicating stable performance across different validation folds. Therefore, RF was selected as the final predictive model because it provided the best balance among prediction accuracy, robustness, and generalization capability.



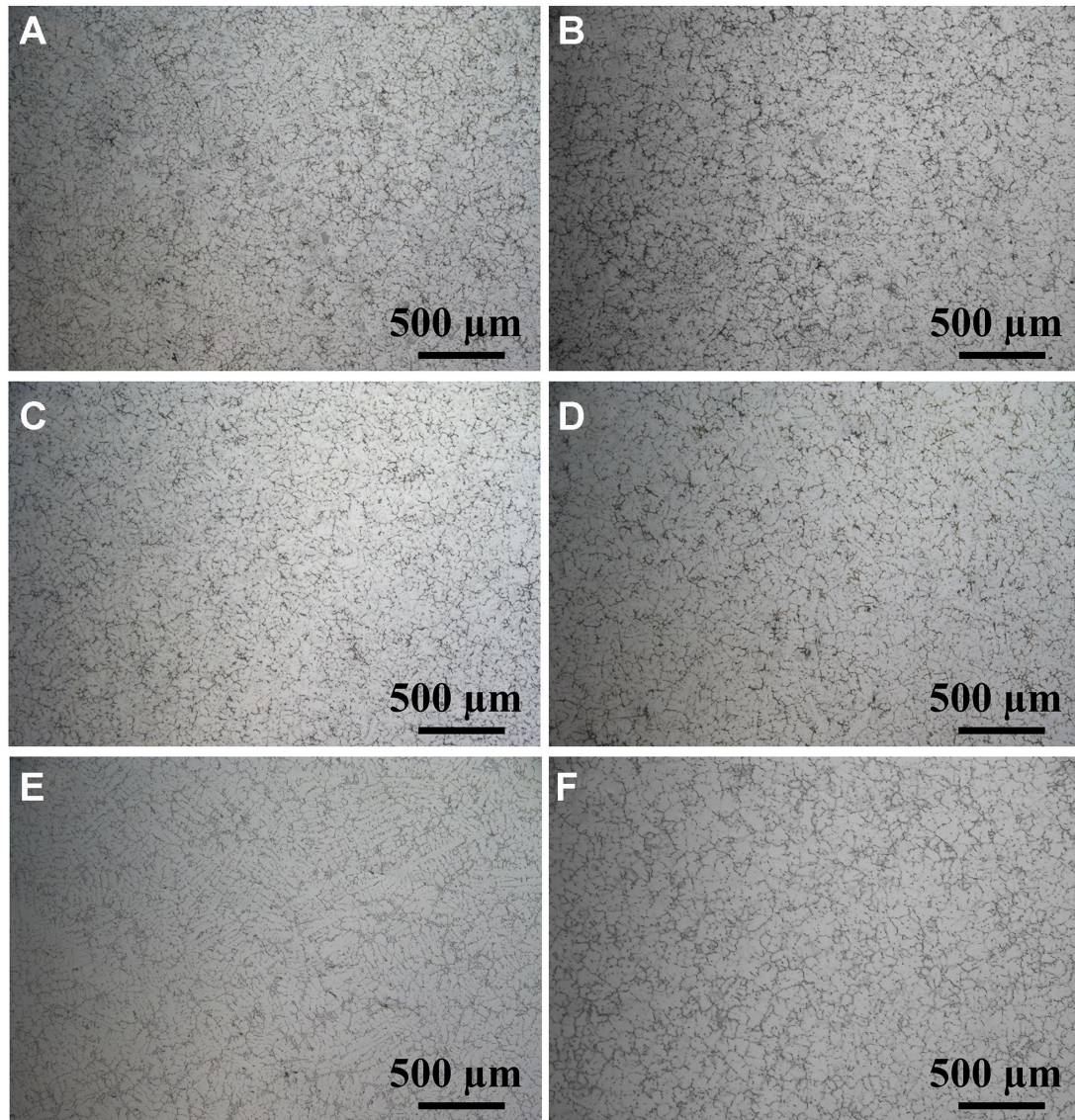
Supplementary Figure 1. Comparison of prediction performance among different regression models.

Comparison of (R^2) values obtained by Random Forest (RF), Gradient Boosting (GB), Extra Trees (ET), support vector regression (SVR), Decision Tree (DT), K-nearest neighbors (KNN), AdaBoost (AdaBoost), Ridge Regression (Ridge), Lasso Regression (Lasso), and Linear Regression (LR) under 10-fold cross-validation and independent test-set evaluation.

Supplementary Table 1. Performance comparison of different regression models based on 10-fold cross-validation and independent test-set evaluation

ML algorithms	10-Fold CV			Test		
	R ²	RMSE	MAE	R ²	RMSE	MAE
RF	0.885±0.023	32.615±3.822	21.505±2.012	0.881	32.944	22.639
GB	0.874±0.029	33.969±4.235	24.400±2.662	0.874	33.847	24.679
ET	0.876±0.024	33.757±3.901	21.231±1.675	0.868	34.732	22.680
SVR	0.798±0.038	43.009±4.063	29.347±1.766	0.799	42.774	30.767
DT	0.824±0.033	40.240±4.263	25.150±2.656	0.785	44.323	28.940
KNN	0.773±0.039	45.792±5.140	32.023±2.614	0.742	48.539	33.711
AdaBoost	0.724±0.033	50.405±2.258	42.023±2.359	0.731	49.574	41.723
Ridge	0.604±0.162	59.604±10.613	45.031±2.367	0.647	56.724	45.328
Lasso	0.604±0.163	59.613±10.626	45.030±2.368	0.647	56.729	45.328
LR	0.604±0.163	59.613±10.627	45.030±2.368	0.647	56.729	45.329

The best value for each evaluation metric is highlighted in bold. Although ET exhibits the lowest 10-fold CV MAE, RF shows the best overall performance considering cross-validation R², cross-validation RMSE, independent test-set accuracy, and generalization stability.



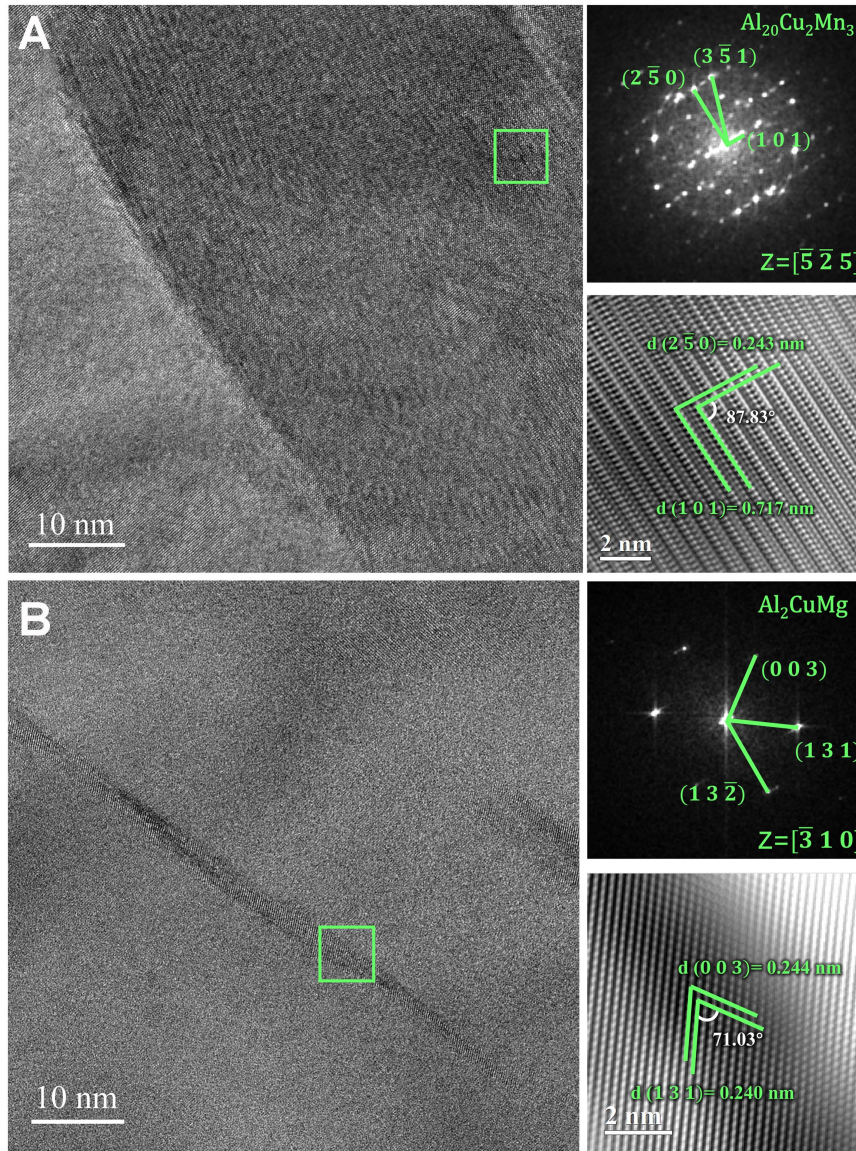
Supplementary Figure 2. Representative as-cast optical micrographs used for secondary dendrite arm spacing (SDAS) measurement of the investigated alloys: (A) ZL-1, (B) ZL-2, (C) ZL-3, (D) ZL-4, (E) ZL114A, and (F) ZL205A.

Note S2. Crystallographic verification of nanoscale precipitates in the ZL-2 alloy

Representative HRTEM images, indexed FFT patterns, and corresponding inverse fast Fourier transform (IFFT) images are presented in Supplementary Figure 3. The FFT patterns were obtained from the precipitate regions marked by green boxes in the HRTEM images.

For the Mn- and Cu-enriched rod-like/plate-like precipitate in Supplementary Figure 3A, the FFT reflections are indexed as the $(2\bar{5}0)$, $(3\bar{5}1)$, and (101) planes along the $[\bar{5}\bar{2}5]$ zone axis. The measured interplanar spacings are 0.243 nm for the $(2\bar{5}0)$ plane and 0.717 nm for the (101) plane, with an interplanar angle of 87.83° , consistent with the reported orthorhombic structure of $\text{Al}_{20}\text{Cu}_2\text{Mn}_3$ [S1]. For the Cu- and Mg-enriched lath-like precipitate in Supplementary Figure 3B, the FFT reflections are indexed as the (003) , (131) , and $(13\bar{2})$ planes along the $[\bar{3}10]$ zone axis. The corresponding interplanar spacings are 0.244 nm for the (003) plane and 0.240 nm for the (131) plane, with an interplanar angle of 71.03° , consistent with the reported orthorhombic structure of Al_2CuMg [S2].

Together with the Mn-Cu and Cu-Mg enrichment revealed by the STEM-EDS elemental maps in Figure 8B and C, respectively, these crystallographic results support the identification of the two precipitate types as Mn-rich $\text{Al}_{20}\text{Cu}_2\text{Mn}_3$ and Al_2CuMg .



Supplementary Figure 3. Crystallographic characterization of representative nanoscale precipitates in the ZL-2 alloy. (A) HRTEM image and corresponding indexed FFT and IFFT images of an Mn- and Cu-enriched $\text{Al}_{20}\text{Cu}_2\text{Mn}_3$ precipitate viewed along the $[\bar{5}\bar{2}5]$ zone axis. (B) HRTEM image and corresponding indexed FFT and IFFT images of a Cu- and Mg-enriched Al_2CuMg precipitate viewed along the $[\bar{3}10]$ zone axis. The green boxes indicate the regions selected for FFT analysis, and the measured interplanar spacings and angles are marked in the corresponding IFFT images.

References

[S1] Shen, Z., Liu, C., Ding, Q., Wang, S., Wei, X., Chen, L., ... & Zhang, Z. The structure determination of $\text{Al}_{20}\text{Cu}_2\text{Mn}_3$ by near atomic resolution chemical mapping. *Journal of alloys and compounds*, 601, 25-30 (2014).

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