Supplemental Information

Yield Strength-Plasticity Trade-off and Uncertainty Quantification for Machine-learning-based Design of Refractory High-Entropy Alloys

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SUPPLEMENTARY INFORMATION

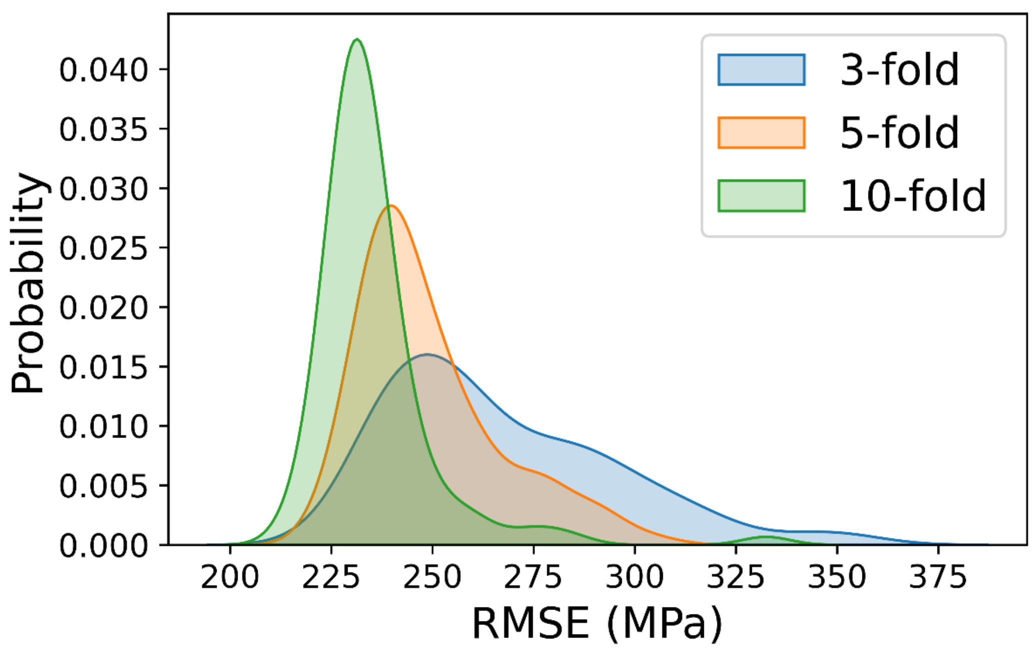

Figure S1. Distribution of error in yield-strength prediction, depicted by kernel density estimate (KDE), for ReLU activation as a function of number of folds.

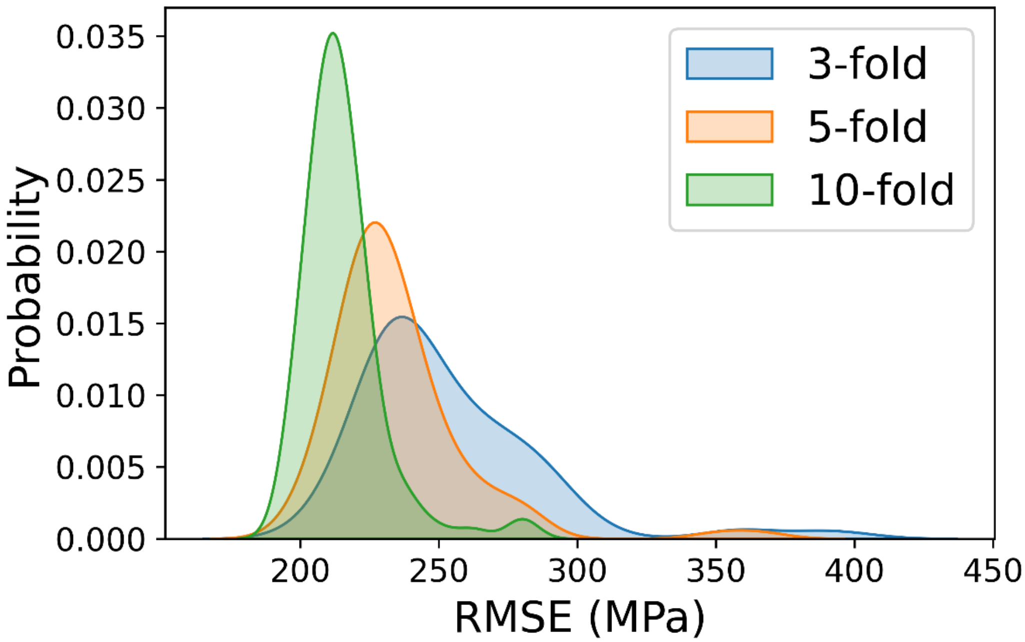

Figure S2. Distribution of error in yield-strength prediction, depicted by KDE, for SELU activation as a function of number of folds.

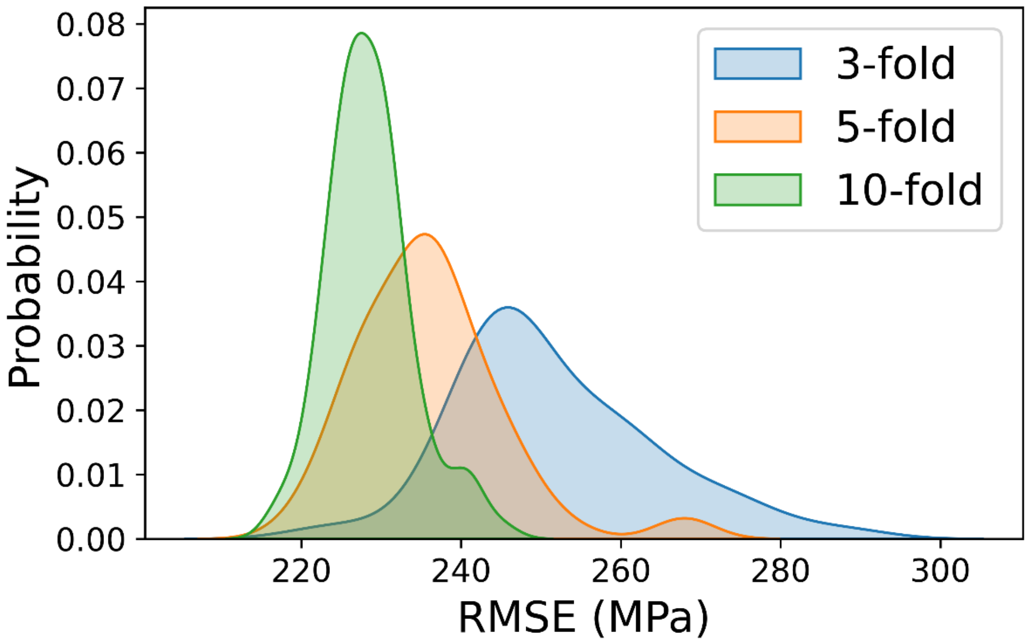

Figure S3. Distribution of error in yield-strength prediction, depicted by KDE, for the random forest model as a function of number of folds.

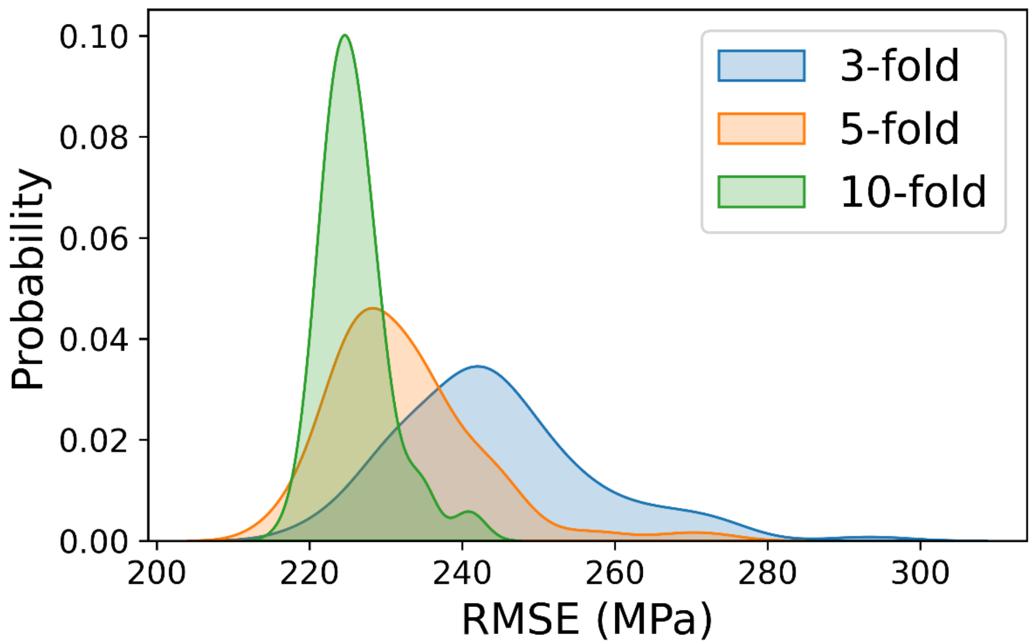

Figure S4. Distribution of error in yield-strength prediction, depicted by KDE, for the gradient-boosting model as a function of number of folds.

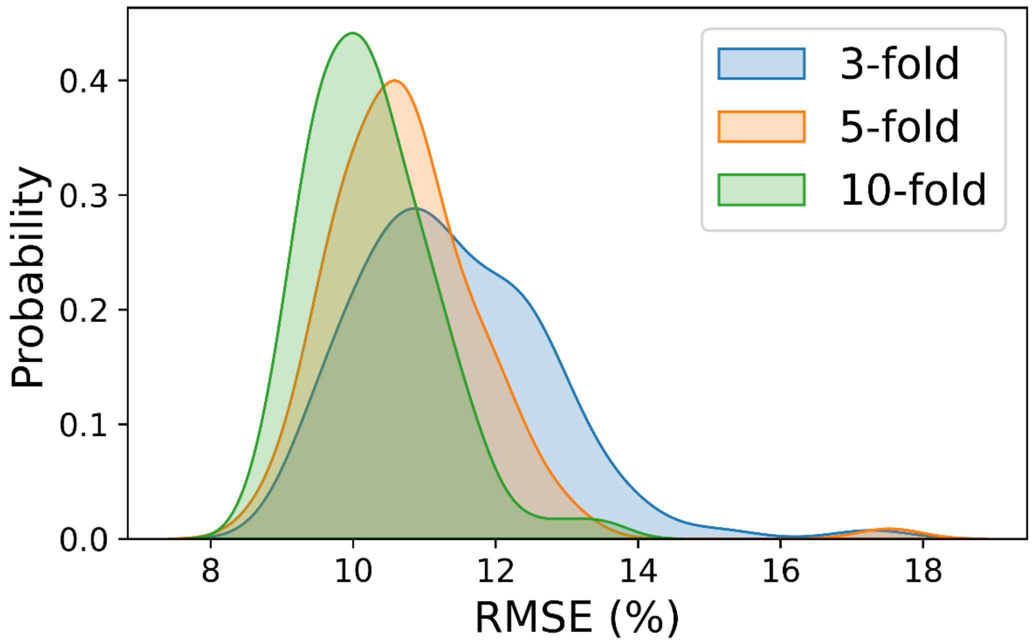

Figure S5. Distribution of error in plasticity prediction, depicted by KDE, for the neural network model with the ReLU activation as a function of number of folds.

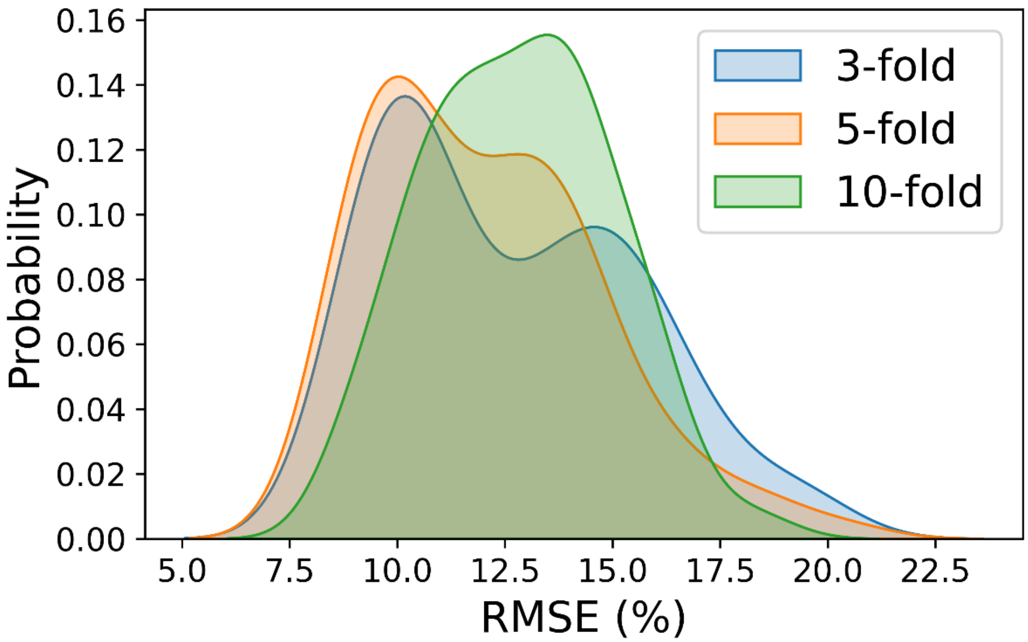

Figure S6. Distribution of error in plasticity prediction, depicted by KDE, for the neural network model with the SELU activation as a function of number of folds.

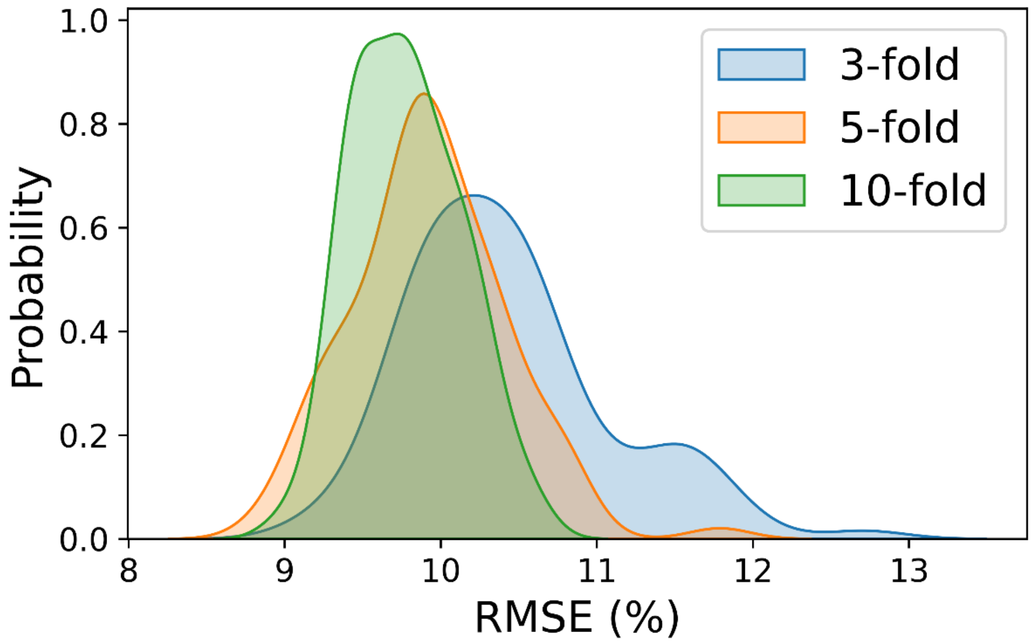

Figure S7. Distribution of error in plasticity prediction, depicted by KDE, for the random-forest model as a function of number of folds.

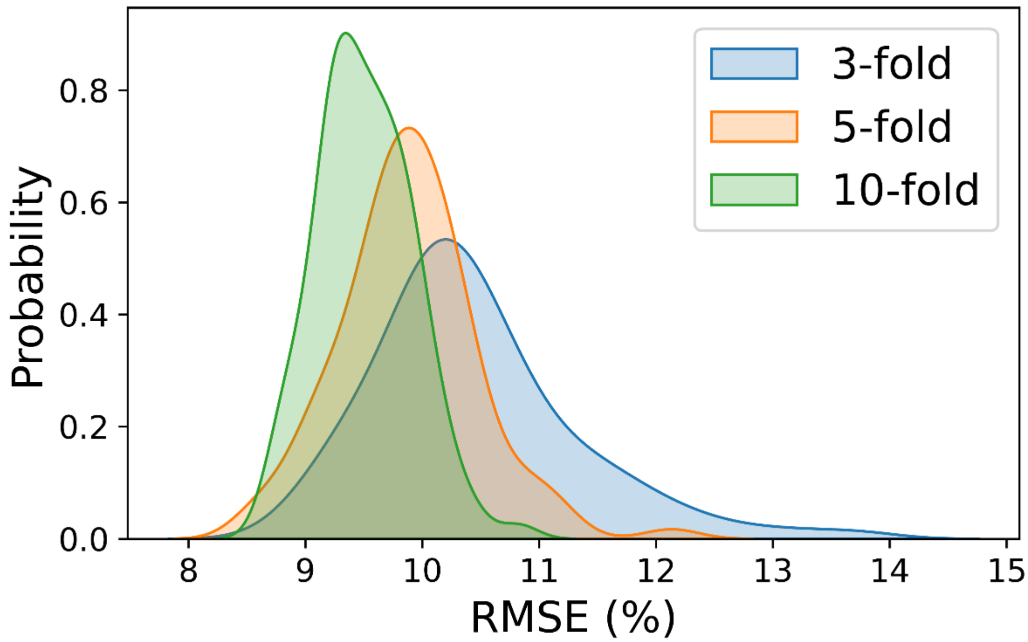

Figure S8. Distribution of error in plasticity prediction, depicted by KDE, for the gradient-boosting model as a function of number of folds.

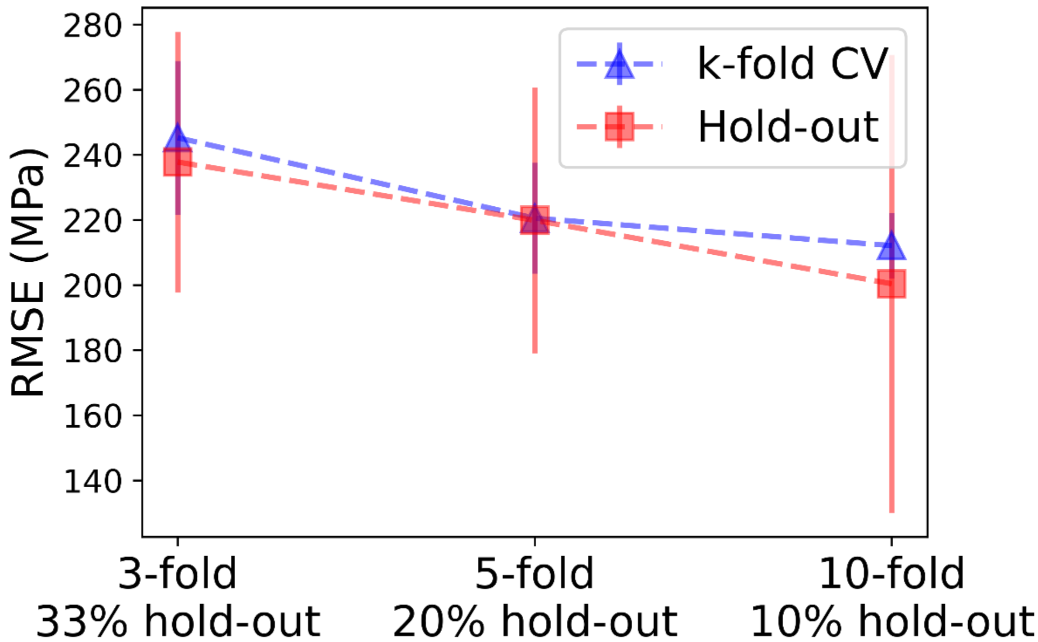

Figure S9. Comparison of *k*-fold cross-validation error estimates to their corresponding hold-out error estimates, where a portion of the dataset has been entirely withheld.

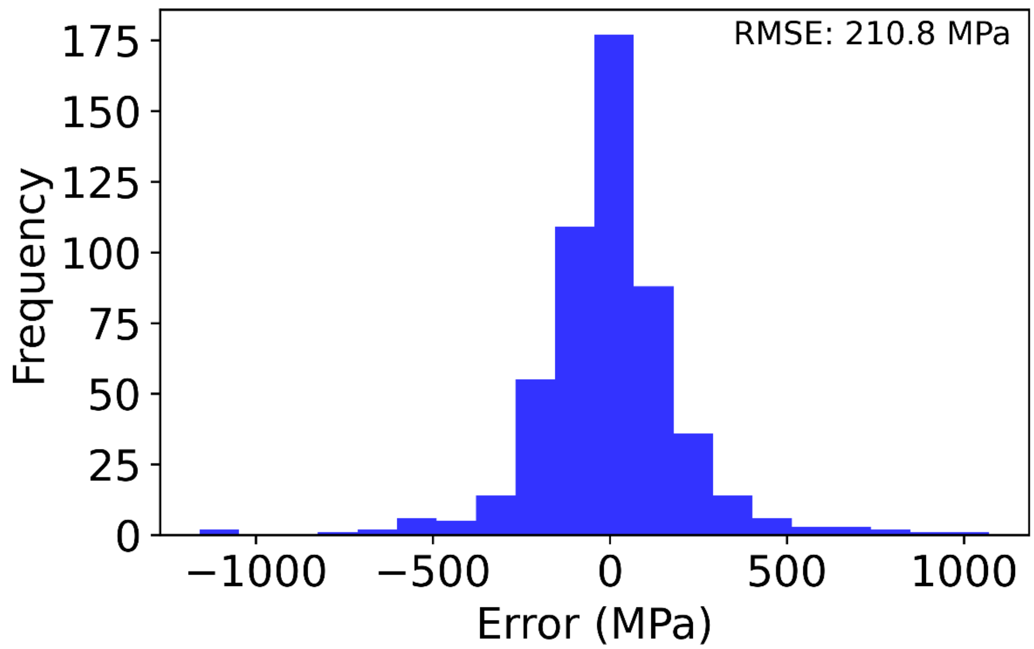

Figure S10. Example error distribution of yield strength for the neural-network model with the Leaky ReLU activation. Errors greater than zero correspond to an overprediction of the true values, whereas errors less than zero correspond to an underprediction.

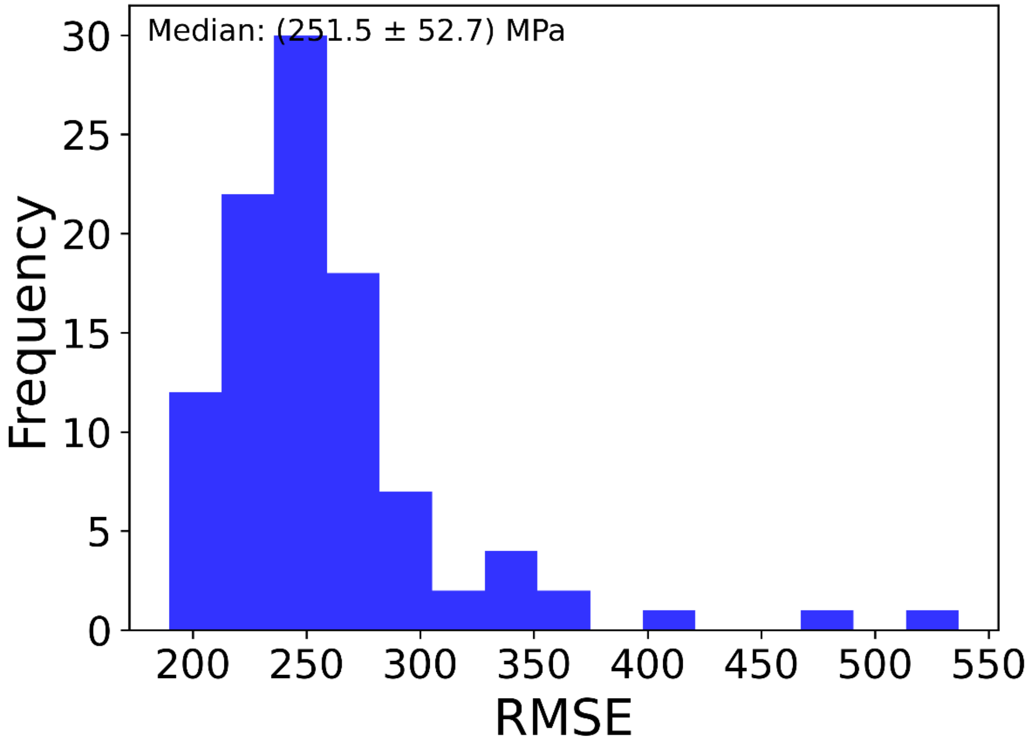

Figure S11. RMSE distribution of the individual bootstrap ensemble models (100 total) as determined by the prediction error for the out-of-bootstrap samples.

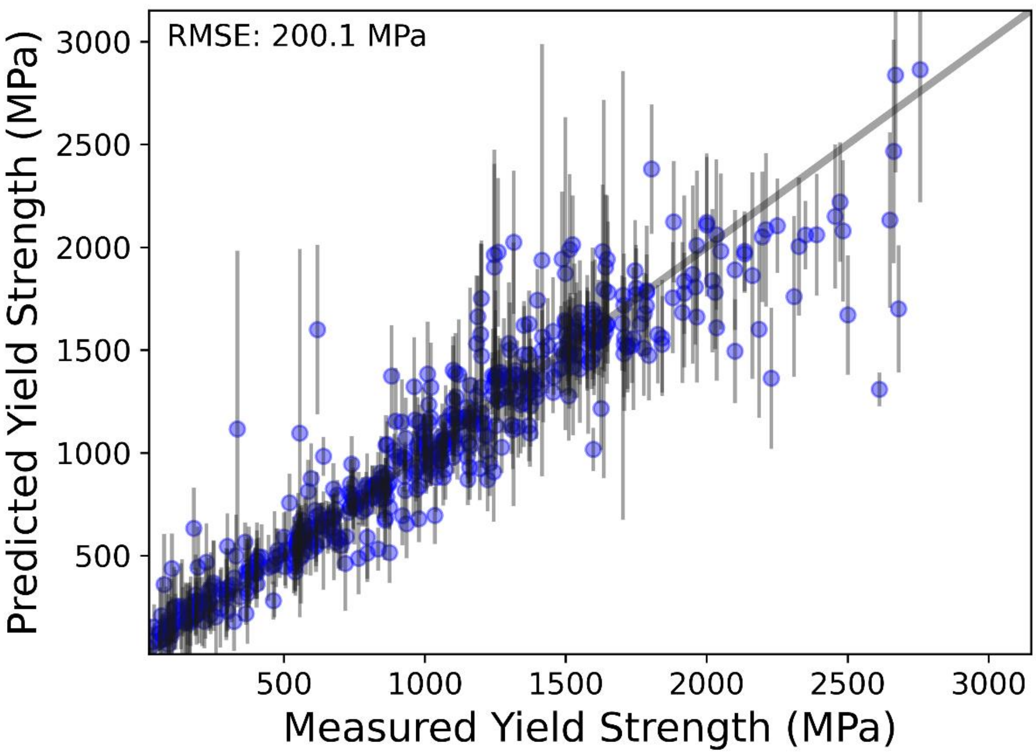

Figure S12. Parity plot of measured and predicted yield strength averaged over the 100 members of the bootstrap ensemble.

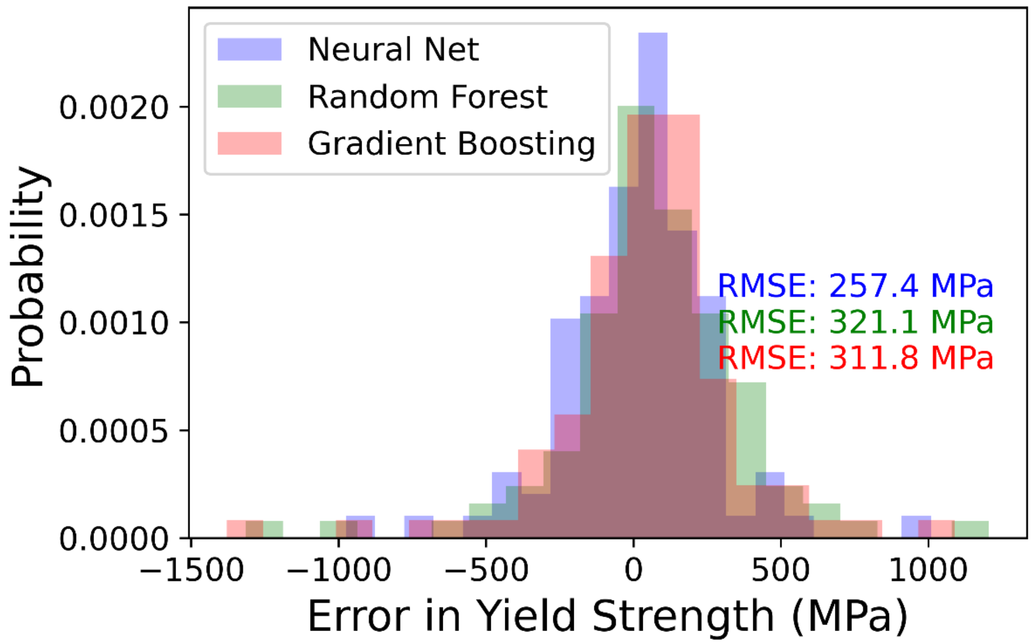

Figure S13. Distribution of the 10-fold cross-validation error in the prediction of unique alloy composition yield strengths for each of the three model types, where the Neural Net results used Leaky ReLU activation.