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INTRODUCTION

We had the great honor of 6th International Conference on Modern and Advanced Research ICMAR 2026. It was truly a great pleasure for us to greet a lot of participants from many different countries to attend ICMAR 2026! We firmly believe that the conference will become an important international event in the field of cross-industry discussion about innovations in Academic Studies.

Three cooperating organizations supported the two-day conference. There were 146 papers accepted for presentation at ICMAR 2026, contributed from different countries. We had plenary speeches and several well-known scientists and experts, to give invited talks at differentsessions.

The purpose of ICMAR 2026 was to provide a forum for the participants to report and review innovative ideas, with up-to-date progress and developments, and discuss novel approaches to the application in the field of their own research areas and discuss challenges of doing science.

We sincerely hope that the exchange of ideas on doing research, science and improving education will help the participants, and international cooperation sharing the common interest will be enhanced.

On behalf the Organization Committee of ICMAR 2026, we would like to heartily thank our cooperating organizations for all they have done for the conference. We would also like to thank the authors for theircontribution to the proceedings; the participants and friends of ICMAR 2026, for their interest and efforts in helping us to make the conference possible; and the Editorial boards for their effective work and valuable advice, especially the ICMAR 2026 secretariat and the ICMAR 2026 staff, for their tireless efforts and outstanding services in preparing the conference and publishing the Proceedings.

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Türkiye dışından toplam 17 farklı ülkeden (Fas, Cezayir, Pakistan, Arnavutluk, Birleşik Krallık, Hindistan, Kosova, Almanya, Azerbaycan, Libya, Nijerya, Irak, Burundi, İtalya, Kuzey Makedonya, Sırbistan, Bangladeş) katılım sağlanmış olup, 146 adet bildirinin 81 (%55,47) tanesi yabancı katılımcı tarafından sunulmuştur.

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Machine and Deep Learning in Mechanics of Materials: The Evaluation Protocol Governs Reported Accuracy in Alloy Yield Strength Prediction

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Abstract – Machine learning is now widely applied to structure and property problems in the mechanics of materials. The accuracy that a study reports, however, depends on how the test set is formed. This work quantifies that dependence for the yield strength of multi-principal element alloys. An open access dataset of 1545 experimental records was used, of which 1067 report both yield strength and test temperature. Eleven composition descriptors were derived from solid solution theory, including atomic size mismatch, mixing entropy and valence electron concentration. Six statistical and machine learning regressors and one deep neural network were trained under three cross-validation protocols. The first protocol shuffles records at random, which is the common practice. The second and the third protocols keep the folds disjoint in alloy composition and in source publication, respectively. A variance component analysis showed that alloy identity explains 64.4 per cent of the yield strength variance, while publication identity explains 61.0 per cent. Random splitting therefore places replicate records of one alloy in the training and the test fold at the same time. Gradient boosting reached a coefficient of determination of 0.796 under random splitting, 0.701 under composition-disjoint splitting and 0.581 under source-disjoint splitting. The deep network followed the same pattern, and the ranking of the models also changed with the protocol. Headline accuracies obtained by random splitting therefore overstate how well a model generalises to an unseen alloy. Grouped validation is recommended whenever a data driven model is intended to support alloy design.

Keywords – High-entropy alloys, yield strength, machine learning, deep learning, cross-validation

I. INTRODUCTION

Data driven methods have become a standard tool in continuum materials mechanics, where they complement constitutive modelling and experiment [1]. Regression models now predict stiffness, strength and ductility directly from composition and processing variables [2]. The appeal is practical, because a surrogate model screens candidate materials far faster than a mechanical test campaign.

Multi-principal element alloys illustrate both the promise and the difficulty of this approach. These alloys contain several elements in near equal proportion, rather than one base element [3], [4]. They can form single phase solid solutions with attractive strength and toughness [5]. Their composition space is enormous, so exhaustive testing is impossible. Empirical descriptors such as the atomic size mismatch, the ideal mixing entropy and the valence electron concentration were introduced to rationalise phase selection [6], [7]. These descriptors are computed from tabulated elemental radii and electronegativities [8]. The same descriptors are now used as machine learning features for property prediction [9].

A question that receives less attention is how such models are validated. Mechanical property datasets are usually compilations assembled from the published literature. One alloy is therefore measured many times, at several test temperatures, and often within a single study. When records are shuffled at random,

replicate measurements of one alloy enter the training fold and the test fold together. The test score then rewards recognition of a familiar alloy rather than genuine extrapolation. This mechanism is a form of data leakage [10]. It has been reported for superconductor discovery [11], for materials discovery campaigns in general [12], and for redundant crystal structure datasets [13]. Its magnitude has not been quantified for the mechanical properties of multi-principal element alloys.

This paper addresses that gap. An open access dataset of experimentally reported alloy properties [14] is combined with descriptors motivated by solid solution mechanics. Six statistical and machine learning regressors and one deep neural network are then evaluated under three cross-validation protocols of increasing strictness. The contributions are threefold. First, the replicate structure of the dataset is quantified by a variance component analysis. Second, the accuracy of every model is reported under random, composition-disjoint and source-disjoint splitting. Third, the effect of the protocol on model ranking is examined. The remainder of the paper is organised as follows. Section II describes the dataset, the descriptors, the models and the protocols. Section III reports the statistical structure and the accuracy results. Section IV discusses the implications for alloy design, and Section V states the conclusions.

II. Materials and Method

This section is organised in five parts. Part A describes the dataset. Part B defines the mechanics based descriptors. Part C lists the regression models. Part D defines the three cross-validation protocols. Part E describes the statistical analysis.

A. Dataset

The study uses the open access compilation of mechanical properties of multi-principal element alloys published by Borg and co-workers [14]. The compilation contains 1545 records extracted from the published literature. Each record reports an alloy composition, a processing route, an observed phase, a test condition and one or more mechanical properties. The present work models the room and elevated temperature yield strength. Records were retained when both the yield strength and the test temperature were reported, which gives 1067 records. These records cover 395 distinct compositions drawn from 191 source publications, and involve 26 chemical elements. Yield strength ranges from 24 to 3416 MPa, and the test temperature ranges from -269 to 1600 degrees Celsius.

B. Mechanics based descriptors

Each formula was parsed into atomic fractions and converted into eleven descriptors that are standard in solid solution theory [6]-[8]. The atomic size mismatch is defined in (1). Here c_i is the atomic fraction of element i, r_i is its atomic radius, and $\bar{r}$ is the composition average radius.

$$\delta = 100 \times [\, \Sigma\, c_i \,(1 - r_i / \bar{r}\,)^2 \,]^{1/2} \qquad (1)$$

The ideal configurational mixing entropy is given in (2), where R is the universal gas constant.

$$\Delta S_{mix} = - R \,\Sigma\, c_i \ln c_i \qquad (2)$$

The remaining descriptors are the number of elements and the mean atomic radius. They also include the rule of mixtures melting point and the valence electron concentration. The mean and the mismatch of Pauling electronegativity complete the chemical set. The mean molar mass and the mean and the mismatch of the elemental shear modulus were added as stiffness proxies. Two test variables follow, namely the test temperature and the homologous temperature. The homologous temperature is the absolute test temperature divided by the rule of mixtures melting point, so it carries the thermal activation argument of deformation mechanics. The reported density, the processing route, the observed phase and the test mode complete the feature set. Table 1 summarises the modelled variables.

C. Regression models

Seven predictors were compared. A mean predictor provides the null reference. Ordinary least squares and ridge regression represent the classical statistical baseline. Support vector regression with a radial basis kernel, a random forest of 500 trees [15] and gradient boosted trees with 600 estimators [16] represent classical machine learning. The deep model is a fully connected network with three hidden layers of 128, 64 and 32 units. It uses batch normalisation, rectified linear activation, dropout of 0.1 and

the Adam optimiser [17]. Training stops early when an inner validation loss stops improving for 40 epochs, and that inner split respects the same grouping as the outer protocol. Hyperparameters were held fixed across all protocols, so that any change in accuracy is caused by the split and not by tuning. The classical models were implemented with scikit-learn [18] and the deep model with PyTorch [19].

D. Cross-validation protocols

Three ten-fold protocols were applied to the same data and the same models. The random protocol shuffles the records, which is the usual practice. The composition-disjoint protocol assigns every record of one alloy composition to a single fold. The source-disjoint protocol assigns every record of one source publication to a single fold. The second protocol therefore tests generalisation to an unseen alloy. The third additionally removes the shared laboratory, the shared processing route and the shared measurement practice of a single study. Each protocol was repeated over five seeds, and the reported values are the mean and the standard deviation across those seeds. All preprocessing was fitted inside the training fold only.

E. Statistical analysis

Descriptive statistics summarise the modelled variables. Spearman rank correlation quantifies the monotone association between each descriptor and the yield strength. The Kruskal-Wallis test compares the yield strength across the reported phase, the processing route and the test mode. A one-way random effects analysis of variance gives the intraclass correlation coefficient for alloy identity and for source identity. That coefficient measures the share of the yield strength variance that lies between groups rather than within them, and it is the statistic that motivates grouped validation.

Table 1. Descriptive statistics of the modelled variables (n = 1067 records).

Variable	Mean	SD	Minimum	Maximum
Yield strength, MPa	890	570	24	3416
Test temperature, C	258	408	-269	1600
Homologous temperature	0.25	0.18	0.00	0.90
Atomic size mismatch, %	4.79	2.15	0.14	19.40
Mixing entropy, J/(mol K)	12.73	1.61	6.44	18.21
Valence electron concentration	6.16	1.69	1.77	9.60
Mean melting point, K	2097	424	702	3261
Mean shear modulus, GPa	66.4	18.1	13.5	116.6
Density, g/cm3	8.08	1.78	1.40	13.70
Number of elements	4.97	0.87	3.00	9.00

III. Results

This section reports the results in three parts. Part A characterises the replicate structure of the dataset. Part B reports the accuracy of every model under the three protocols. Part C examines the effect of the protocol on model ranking.

A. Replicate structure and descriptive statistics

The 1067 modelled records describe only 395 distinct compositions. A composition that appears more than once accounts for 76.3 per cent of the records, and the largest single composition contributes 40 records. The corresponding figures for source publications are 96.9 per cent and 78 records. Repetition is not simple duplication, because the median spread of test temperature within a repeated composition is 775 degrees Celsius. The one-way analysis of variance gives an intraclass correlation of 0.437 for alloy identity and 0.529 for source identity, both with p below 0.001. Group identity alone explains 64.4 per cent of the yield strength variance for compositions and 61.0 per cent for sources. Fig. 1 shows the resulting replication structure and the strength distribution.

The descriptive statistics of the modelled variables are given in Table 1. Two mechanics effects are visible in the raw data. The test mode separates the population, because the median yield strength is 1010 MPa in compression and 521 MPa in tension. A Mann-Whitney test confirms the difference, with p below

0.001 and a Cliff delta of 0.41. The reported phase also matters, since body centred cubic alloys are stronger and less ductile than face centred cubic alloys. Fig. 1(b) displays both effects.

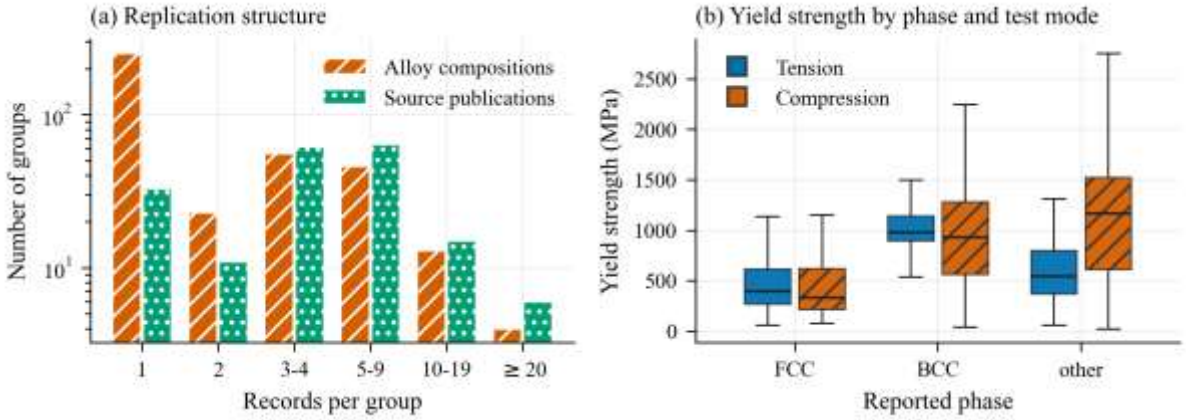


Fig. 1 Structure of the modelled dataset. (a) Number of records per alloy composition and per source publication. (b) Yield strength by reported phase and test mode.

B. Accuracy under the three protocols

Table 2 reports the coefficient of determination and the root mean squared error for every model and protocol. Under random splitting the best model is gradient boosting, which reaches an R squared of 0.796. That value is the kind of headline number usually reported for this class of problem. The same model and the same hyperparameters give 0.701 when the folds are disjoint in composition and 0.581 when they are disjoint in source. The loss of explained variance is therefore 0.095 and 0.215, respectively. The root mean squared error rises from 257 MPa to 369 MPa over the same comparison. The deep network behaves in the same way, falling from 0.793 to 0.613, a loss of 0.179. Fig. 2 shows the effect for every model, and Fig. 3 shows the corresponding parity plots.

Table 2. Out-of-fold accuracy by model and cross-validation protocol. Values are the mean over five seeds, with the standard deviation in brackets. RMSE is in MPa.

Model	Random		Composition-disjoint		Source-disjoint	
	R^2	RMSE	R^2	RMSE	R^2	RMSE
Mean baseline	-0.002 (0.001)	571	-0.007 (0.001)	572	-0.007 (0.004)	572
Linear regression	0.589 (0.002)	365	0.565 (0.007)	376	0.525 (0.015)	393
Ridge regression	0.589 (0.002)	366	0.569 (0.004)	374	0.536 (0.012)	388
Support vector regression	0.685 (0.003)	320	0.644 (0.002)	340	0.616 (0.006)	353
Random forest	0.786 (0.008)	264	0.681 (0.009)	322	0.570 (0.016)	373
Gradient boosting	0.796 (0.008)	257	0.701 (0.011)	311	0.581 (0.019)	369
Deep neural network	0.793 (0.007)	260	0.671 (0.022)	327	0.613 (0.028)	354

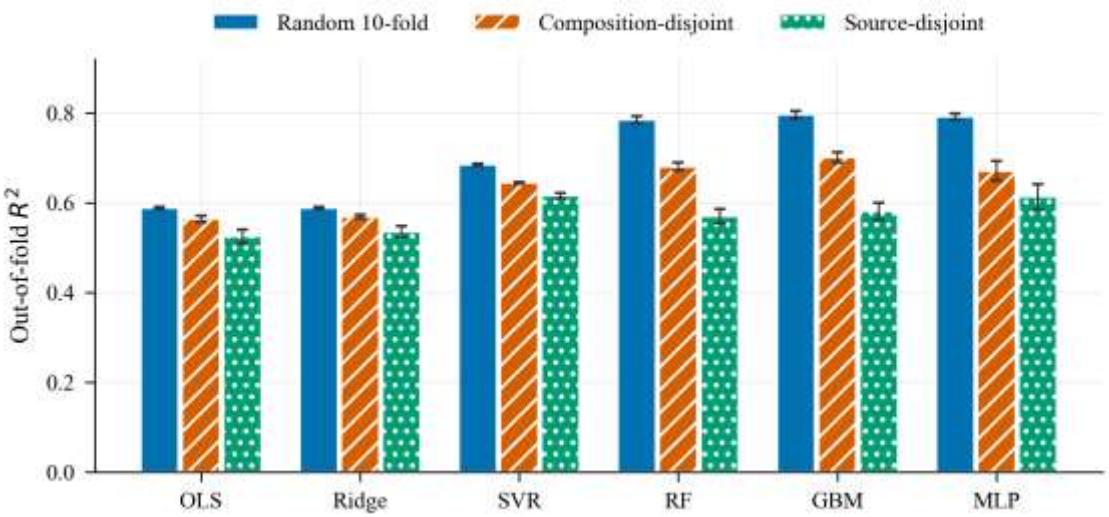


Fig. 2 Out-of-fold coefficient of determination for each model under the three cross-validation protocols. Bars are the mean over five seeds and error bars are one standard deviation.

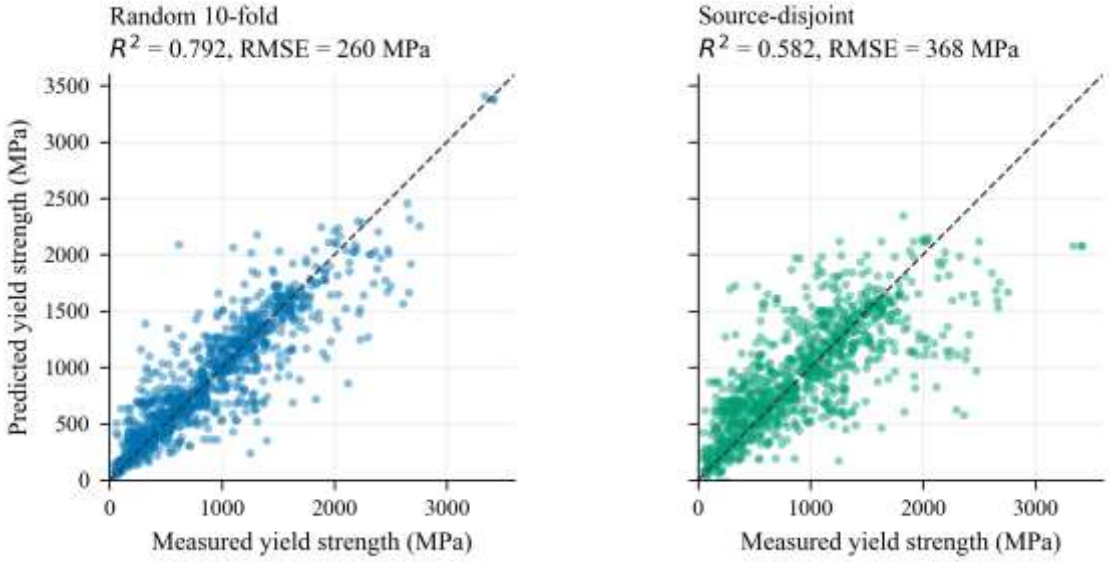


Fig. 3 Out-of-fold parity plots for gradient boosting under the loosest and the strictest protocol. The dashed line is the ideal prediction.

C. Effect of the protocol on model ranking

The protocol also changes which model appears best. Under random splitting the ranking is led by gradient boosting, followed by deep neural network. Under source-disjoint splitting the leader is support vector regression. The gap between the flexible learners and the linear baseline narrows sharply. The flexible learners lose the most when replicate records leave the training fold. Linear regression reaches 0.525 under the strictest protocol, against 0.589 under random splitting. A comparison made under random splitting would therefore recommend a different model from the one that generalises best to an unseen alloy.

In summary, the results establish three findings. Alloy identity and source identity explain most of the yield strength variance. Random splitting inflates the reported accuracy of every learned model, and the inflation is largest for the most flexible models. The choice of protocol also alters the ranking of the models.

IV. Discussion

The results show that the evaluation protocol, and not only the learning algorithm, determines the accuracy that a study reports. The mechanism is specific to the way mechanical property datasets are

built. A literature compilation records one alloy many times, at several test temperatures and often inside one study. Random splitting then asks the model to interpolate between two measurements of a material it has already seen. That task is much easier than predicting the strength of a new alloy, which is the task that alloy design actually requires.

The variance component analysis explains why the effect is so large. Group identity accounts for the majority of the yield strength variance, so knowing the alloy is close to knowing the answer. This observation agrees with reports from other branches of materials informatics, where clustered validation and redundancy control produced similar reductions [11], [13]. The present study adds a quantitative estimate for the mechanical properties of multi-principal element alloys, and it separates two distinct grouping levels. The source-disjoint protocol is the stricter of the two, which indicates that a shared laboratory and a shared processing route leak information beyond composition alone.

The practical implication is not that machine learning fails in mechanics of materials. The models still explain a useful share of the variance under the strict protocols, and they remain far better than the mean predictor. The implication is that a headline score obtained by random splitting is the wrong quantity to report when the intended use is design. A grouped score answers the question that a designer asks, which is how the model will behave on an alloy that has never been tested. Reporting both values is inexpensive and makes the claim verifiable.

Three limitations should be stated. The dataset mixes tension and compression tests, and the two populations differ significantly, so the test mode was included as a feature rather than modelled separately. Hyperparameters were fixed rather than tuned inside each protocol, which keeps the comparison controlled but may understate the achievable accuracy. Finally, the descriptors are composition averages, so they do not capture grain size, texture or precipitate state, all of which govern strength in real microstructures.

V. Conclusion

This study combined an open access dataset of multi-principal element alloys with descriptors from solid solution mechanics, and evaluated seven regression models under three cross-validation protocols. The main conclusions are the following.

1) Alloy identity explains 64.4 per cent and source identity explains 61.0 per cent of the yield strength variance, so the records are strongly replicated.

2) Gradient boosting falls from an R squared of 0.796 under random splitting to 0.701 under composition-disjoint splitting and 0.581 under source-disjoint splitting.

3) The deep neural network shows the same loss, so the effect is a property of the evaluation protocol and not of one model family.

4) The ranking of the models changes with the protocol, so a model chosen under random splitting need not be the model that generalises best.

5) Grouped validation should be reported whenever a data driven model in mechanics of materials is intended to guide the design of a new material.

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