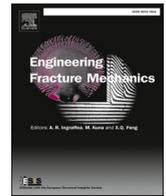




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A new artificial neural network model for prediction of fatigue strength and yield strength of various steel grades[☆]

Dj. Ivković^{a,*} , D. Arsić^a , D. Adamović^a , A. Sedmak^b , M. Delić^a, R. Vulović^c

^a Faculty of Engineering, University of Kragujevac, Kragujevac, Serbia

^b Faculty of Mechanical Engineering, University of Belgrade, Kraljice Marije 16, Belgrade, Serbia

^c Institute for Information Technologies, University of Kragujevac, Jovana Cvijića bb, Kragujevac, Serbia

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ABSTRACT

The prediction of mechanical properties of steels traditionally relies on experimental testing and empirical modeling, which are time-consuming and resource-intensive. Recent advances in artificial intelligence (AI) and machine learning (ML) enable efficient estimation of material properties directly from chemical composition data. In this study, two Artificial Neural Network (ANN) models were developed to predict key mechanical properties of steels—fatigue strength and yield strength—using chemical composition as the sole input. Each network employed a feed-forward backpropagation architecture with Bayesian regularization and was trained on a dataset comprising 200 steel grades, including structural, high-strength, and tool steels. The models were evaluated through regression analysis and further validated using experimental data for three representative steels: S355J2 + N, S690QL, and X37CrMoV5-1. The fatigue strength model achieved correlation coefficients of $R = 0.895$ (training), 0.833 (validation), and 0.893 (testing), with an average prediction error of approximately 9%. The yield strength model reached $R = 0.835$ (training), 0.829 (validation), and 0.864 (testing), with a mean absolute percentage error of 3.97%. The obtained results demonstrate that ANN-based models can reliably capture the relationship between chemical composition and mechanical properties of steels, supporting preliminary material screening and property estimation. The proposed approach provides a basis for the development of data-driven tools in digital materials engineering.

1. Introduction

The development of modern materials and metal processing technologies largely depends on the ability to accurately assess mechanical properties. Traditional approaches, including experimental testing and analytical–empirical models, remain fundamental in engineering practice; however, they are time-consuming, resource-intensive, and often require complex sample preparation. In contrast, the increasing availability of materials data and rapid advances in computational technologies have enabled the application of Artificial Intelligence (AI) and Machine Learning (ML) in engineering sciences, allowing fast and accurate prediction of material properties while significantly reducing the need for extensive experimental campaigns.

Among various machine learning approaches, Artificial Neural Networks (ANN) have been widely applied in materials engineering

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* Corresponding author.

E-mail address: djordje.ivkovic@fink.rs (Dj. Ivković).

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Nomenclature

Symbol/Abbreviation	Definition
ANN	Artificial Neural Network
AI	Artificial Intelligence
ML	Machine Learning
R	Regression coefficient
MAPE	Mean Absolute Percentage Error
n	Number of neurons
f(x)	Output function
w	Connection weight
b	Bias term
BR	Bayesian Regularization algorithm
TANSIG	Hyperbolic tangent sigmoid activation function
CES	Cambridge Engineering Selector
MPa	Megapascal

to capture complex, nonlinear relationships between material composition, processing parameters, and mechanical properties [1,2]. Compared to traditional regression approaches, Artificial Neural Networks (ANN) are particularly effective in capturing nonlinear relationships without requiring predefined analytical expressions. This makes them well suited for complex metallurgical systems, where mechanical properties result from the interaction of multiple interrelated factors [1–4].

Artificial Neural Networks have been extensively applied in materials engineering to predict static and fatigue-related mechanical properties of steels using data-driven approaches. Several studies demonstrated the capability of ANN models to estimate material-related variables based on chemical composition, including ferritic steels [5], C–Mn cast steels [8], and stainless steels [9], achieving satisfactory agreement with experimental results. In addition to composition-based models, ANN approaches have also been employed using process-related or derived parameters, such as Jominy distance for hardness prediction in low-alloy steels [6] and process variables influencing mechanical behavior of dual-phase steels [7]. Furthermore, hybrid ANN-based models have been proposed to enhance prediction accuracy for time-dependent properties, such as creep life of high-temperature steels [10]. Beyond mechanical property prediction, ANN methods have also been successfully applied to other metallurgical problems, including formability assessment and dimensional change prediction during processing [11,12]. Despite these advances, most existing studies focus on specific steel families or single mechanical properties, while comprehensive data-driven frameworks employing separate ANN models to predict different classes of mechanical properties across a wide range of steel grades using chemical composition as the sole input remain limited.

The aim of this study is to develop and analyze two independent Artificial Neural Network models for predicting key mechanical properties of steels—fatigue strength and yield strength—using chemical composition as the sole input. Each ANN model is trained separately for a specific property while sharing a unified input framework, enabling a consistent comparison of predictive performance across different classes of mechanical behavior. The proposed approach covers a wide range of steel grades, including structural, high-strength, and tool steels, rather than being limited to a single steel family. The predictive capability of both models is evaluated using regression analysis and validated by comparison with experimentally determined fatigue strength and yield strength values for three representative steels: S355J2 + N, S690QL, and X37CrMoV5-1. The obtained results demonstrate the potential of composition-based ANN models as effective tools for preliminary material screening and rapid property assessment in the early stages of alloy design.

2. Methodology

2.1. Data selection and preparation

The dataset used in this study was compiled from the Cambridge Engineering Selector (CES) EduPack 2010 materials database, which provides mechanical properties and chemical compositions for a wide range of steel grades. Approximately 200 steel grades were selected, covering structural, high-strength quenched-and-tempered, and tool steels, thereby ensuring a broad representation of alloy systems and mechanical behavior.

For both Artificial Neural Network models, the input parameters consisted of the chemical composition expressed as mass fractions of 18 alloying elements (e.g., C, Mn, Si, Cr, Ni, Mo). Due to the diversity of steel groups included in the dataset, not all alloying elements were present in each steel grade. In such cases, the mass fraction of absent elements was set to zero in order to maintain a consistent input vector dimension across all samples.

Two independent output datasets were defined: fatigue strength for the first ANN model and yield strength for the second ANN model. All input and output data were normalized to the range [0,1] to prevent dominance of variables with larger numerical values and to improve numerical stability and convergence during network training.

It should be noted that the dataset does not explicitly include information on heat treatment conditions, surface state, or microstructural features. Consequently, the chemical composition serves as a surrogate descriptor that implicitly reflects typical processing

routes associated with each steel grade. This limitation is considered in the interpretation of the results and defines the intended application of the proposed models as preliminary screening tools rather than final design predictors.

2.2. Artificial Neural Networks

2.2.1. Artificial Neural Network for predicting fatigue strength

For the prediction of fatigue strength of steels, a feed-forward backpropagation Artificial Neural Network with Bayesian regularization was developed. The input vector consisted of 18 chemical elements representing the alloy composition, while the single output variable was fatigue strength, expressed in MPa. To ensure a consistent input structure, alloying elements not present in a given steel grade were assigned a zero mass fraction. The dataset comprised approximately 200 steel grades extracted from the CES EduPack 2010 database and was normalized to the range [0,1]. The data were randomly divided into training (70%), validation (15%), and testing (15%) subsets.

Bayesian regularization was employed as the training algorithm in order to improve generalization capability and to control model complexity, which is particularly important when dealing with a limited number of samples and a relatively high-dimensional input space. Hyperbolic tangent sigmoid activation functions were used in the hidden and output layers. Model performance was evaluated using the regression coefficient (R) and mean square error (MSE).

Several ANN architectures were examined to identify a stable and accurate configuration. The number of hidden neurons was varied between 5 and 25, and networks with one to three hidden layers were tested. The results indicated that a single hidden layer provided superior convergence stability and reduced overfitting compared to deeper architectures, while increasing the number of neurons beyond approximately 10 did not lead to further improvement in prediction accuracy. Consequently, a network with one hidden layer and 10 neurons was selected as an optimal compromise between accuracy, robustness, and computational efficiency (Fig. 1).

To reduce the influence of random weight initialization, the training procedure was repeated multiple times with different initial conditions, and the reported performance represents the typical behavior of the optimized network. This approach ensures that the obtained results reflect the general predictive capability of the model rather than a single deterministic training outcome.

Table 1 summarizes the main training parameters of the proposed ANN model. The selected hyperparameters were chosen to ensure stable convergence and robust generalization. Bayesian regularization was employed to effectively control overfitting without the need for an explicit early stopping criterion. The maximum number of training epochs was set to 1000, with a minimum performance gradient of 1×10^{-7} to ensure numerical convergence. A low momentum value (0.001) was adopted to promote stable weight updates and to reduce oscillations during training.

In addition to the fatigue strength prediction model, a second, independently trained Artificial Neural Network was developed for estimating yield strength values. Although both models share the same input structure based on chemical composition, they were trained separately to account for the fundamentally different nature of fatigue-related and static mechanical properties. This dual-network approach enables a consistent comparison of ANN predictive performance across different classes of mechanical behavior under identical input conditions.

2.2.2. Artificial Neural Network for predicting yield strength values

A second, independently trained Artificial Neural Network was developed to predict the yield strength of steels. Although the input structure was identical to that of the fatigue strength model—consisting of mass fractions of 18 alloying elements—the yield strength ANN was trained separately to account for the fundamentally different nature and variability of static mechanical properties. The output variable of this network was yield strength, expressed in MPa.

The dataset comprised the same set of approximately 200 steel grades extracted from the CES EduPack 2010 database and was normalized to the range [0,1]. The data were randomly divided into training (70%), validation (15%), and testing (15%) subsets. Bayesian regularization was employed as the training algorithm to improve generalization and to control model complexity, while hyperbolic tangent sigmoid activation functions were used in the hidden and output layers. Model performance was assessed using the regression coefficient (R) and mean square error (MSE).

The separation of fatigue strength and yield strength prediction into two independent ANN models avoids the use of a single multi-output network and allows each model to specialize in learning property-specific relationships between chemical composition and mechanical response. This strategy improves robustness and interpretability of the predictions and enables a consistent comparison of ANN performance for fatigue-related and static properties under identical input conditions. The final architecture of the yield strength ANN is presented in Fig. 2.

To ensure stable and representative results, the training procedure was repeated multiple times using different initial weight

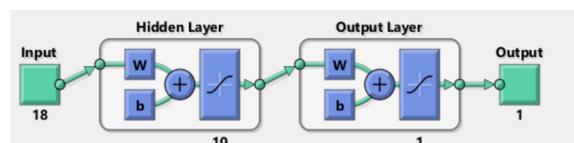


Fig. 1. Architecture of the ANN for predicting fatigue strength values.

Table 1
Main parameters of first ANN.

Parameter	Description
Network type	Feed-forward backpropagation
Training algorithm	Bayesian regularization
Learning function	learnqdm (gradient descent momentum)
Input parameters	18 chemical elements
Output parameters	Fatigue strength, MPa
Number of hidden layers	1
Number of neurons	10
Activation functions	Hidden layer: tansig, Output layer: tansig
Training/ validation/ test ratio	70/15/15%
Momentum	0.001
Evaluation metrics	R

configurations, and the reported performance reflects the typical behavior of the optimized network.

Table 2 summarizes the main training parameters of the ANN model developed for yield strength prediction. The number of training epochs and convergence criteria were kept consistent with those used for the fatigue strength network in order to ensure methodological consistency. Low momentum values and hyperbolic tangent sigmoid activation functions were adopted to promote stable convergence and robust generalization during training.

Both ANN models share a common input structure and a consistent training methodology, which enables a direct and meaningful comparison of predicted fatigue strength and yield strength under identical input conditions. The predictive capability of both networks was evaluated by comparison with experimentally measured mechanical properties of selected steel grades, providing a reliable basis for assessing the applicability of the proposed approach.

3. Results

This section presents the results obtained from the evaluation of the developed Artificial Neural Network (ANN) models for predicting the mechanical properties of steels. The analysis focuses on two independently trained models: one designed for fatigue strength prediction and the other for yield strength estimation. The performance of each network was assessed using regression analysis and correlation coefficients (R) by comparing the predicted values with experimental data.

3.1. ANN model for fatigue strength prediction

The predictive performance of the ANN developed for fatigue strength estimation was evaluated using regression analysis and comparison between predicted and experimental values. The analysis was conducted on the complete dataset as well as on three representative steel grades, enabling assessment of both overall model performance and practical predictive capability. The corresponding regression plots are presented in Figs. 3 and 4. Although a linear regression fit is shown for visualization purposes, the correlation coefficients were evaluated with respect to the bisector line ($Y = T$), ensuring that the reported values reflect prediction accuracy rather than fitting quality.

The obtained correlation coefficients were $R = 0.895$ for the training set, $R = 0.833$ for the validation set, $R = 0.893$ for the testing set, and $R = 0.867$ for the complete dataset. These results indicate a strong correlation between predicted and experimental fatigue strength values, confirming that the ANN successfully captured the nonlinear dependence of fatigue strength on chemical composition. The comparable R values for the training and testing subsets suggest stable generalization behavior without evident overfitting.

Further validation was performed by comparing ANN predictions with experimentally determined fatigue strength values for three representative steel grades: S355J2 + N, S690QL, and X37CrMoV5-1. The predicted values are compared with experimental results in Table 3. The differences between predicted and experimental fatigue strength values were 18.6 MPa (9.3%), 37.2 MPa (12.4%), and -25.2 MPa (5.0%) for S355J2 + N, S690QL, and X37CrMoV5-1, respectively. The average absolute deviation of approximately 9% demonstrates satisfactory predictive accuracy across different steel groups. A slight positive bias was observed, which can be attributed to the limited dataset size and the diversity of steel grades included.

The Fig. 5 illustrates the agreement between predicted and experimental values and highlights the magnitude of deviations for each steel grade.

The comparison between predicted and experimental fatigue strength values demonstrates that the developed ANN model provides

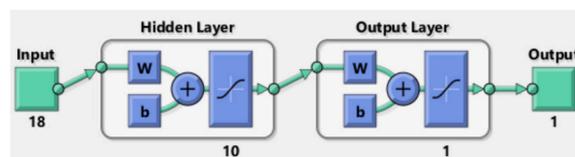


Fig. 2. Architecture of the ANN for yield strength values.

Table 2
Main parameters of second ANN.

Parameter	Description
Network type	Feed-forward backpropagation
Training algorithm	Bayesian regularization
Learning function	learngdm (gradient descent momentum)
Input parameters	18 chemical elements
Output parameters	Yield strength, MPa
Number of hidden layers	1
Number of neurons	10
Activation functions	Hidden layer: tansig, Output layer: tansig
Training/ validation/ test ratio	70/15/15%
Momentum	0.005
Evaluation metrics	R

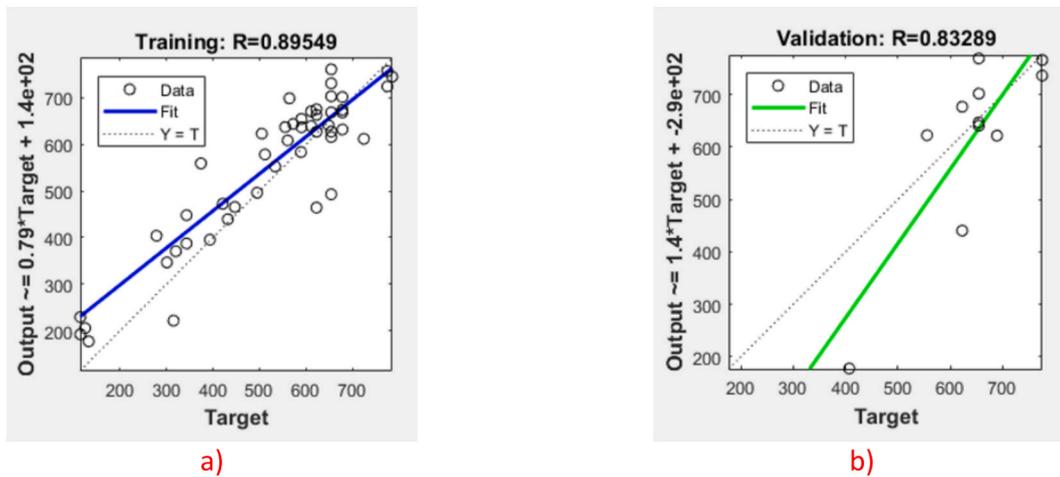


Fig. 3. A) comparison between predicted and experimental fatigue strength values obtained by the ann model for the training dataset. b) comparison between predicted and experimental fatigue strength values obtained by the ann model for the validation dataset.

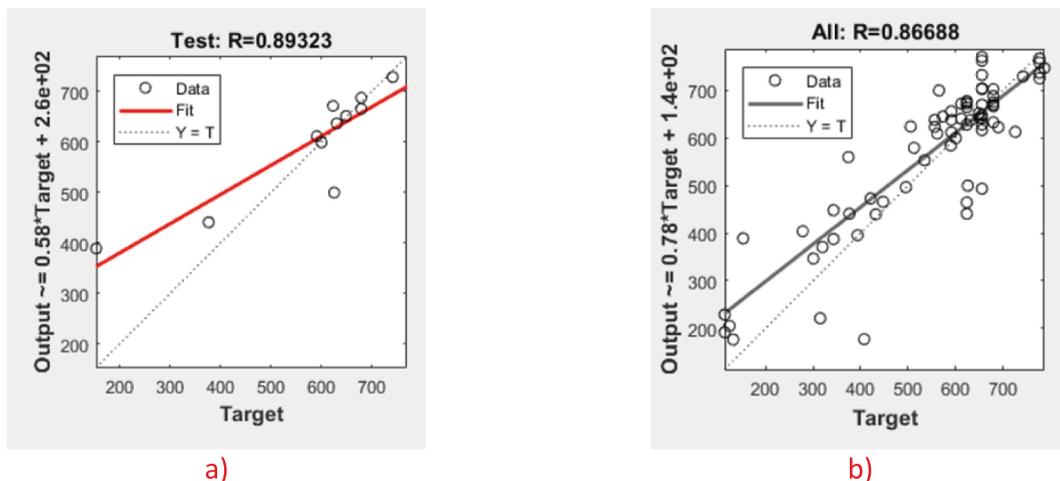


Fig. 4. A) comparison between predicted and experimental fatigue strength values obtained by the ann model for the testing dataset b) comparison between predicted and experimental fatigue strength values obtained by the ann model for the complete dataset.

satisfactory accuracy for all analyzed steel grades. For S355J2 + N, S690QL, and X37CrMoV5-1, the differences between experimental and predicted fatigue strength values were 18.6 MPa (9.3%), 37.2 MPa (12.4%), and - 25.2 MPa (5.0%), respectively. The average absolute deviation of approximately 9% indicates that the network successfully generalized the relationship between chemical

Table 3
Comparison between estimated and experimental fatigue strength values [13].

Steel grade	S355J2 + N	S690QL	X37CrMoV5-1
Estimated value	218.58	337.17	474.84
Experimental value	200	300	500
Error value, MPa	18.58	37.17	25.16
Error, %	9.29	12.39	5.03

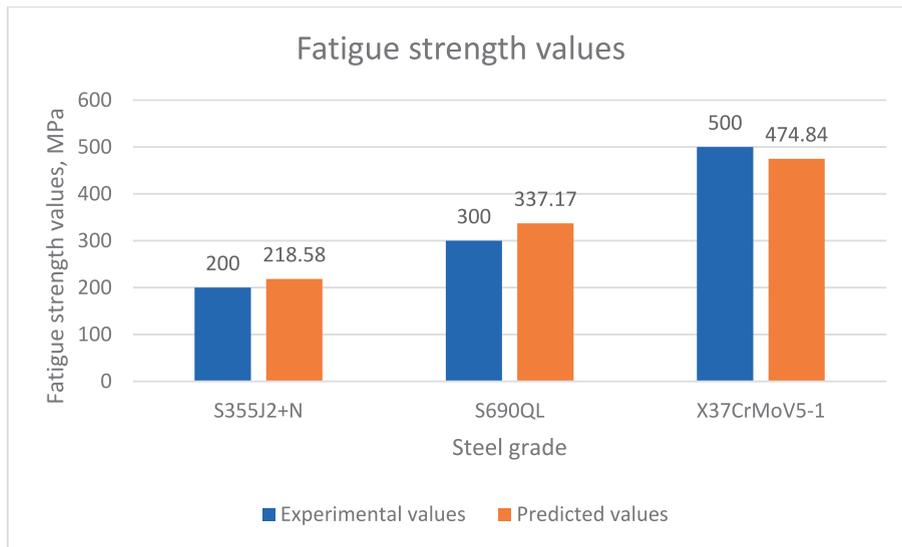
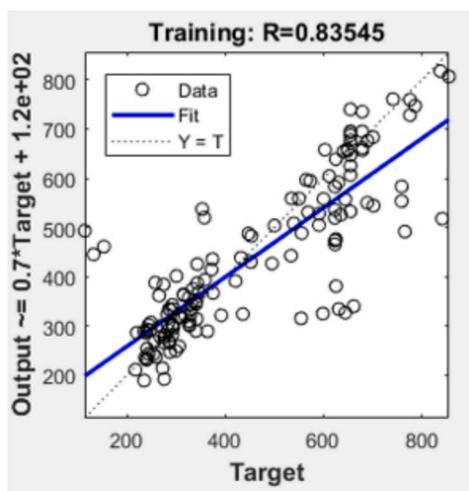
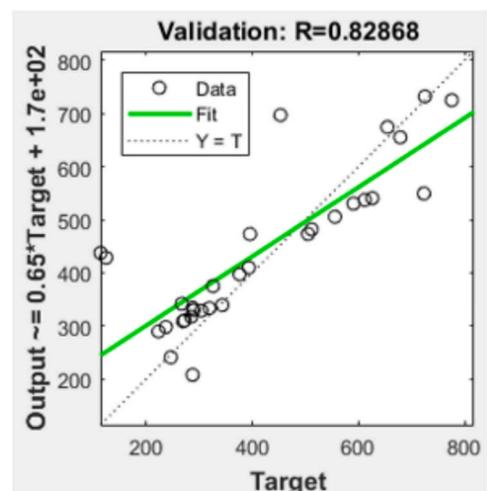


Fig. 5. Comparison between experimentally measured and ANN-predicted fatigue strength values for three representative steel grades: S355J2 + N, S690QL, and X37CrMoV5-1.



a)



b)

Fig. 6. A) comparison between predicted and experimental yield strength values obtained by the ann model for the training dataset b) comparison between predicted and experimental yield strength values obtained by the ann model for the validation dataset.

composition and fatigue strength across different steel groups. A slight positive bias was observed in the predictions, which can be attributed to the limited dataset size and the diversity of steel grades included.

3.2. ANN model for yield strength prediction

The predictive performance of the ANN developed for yield strength estimation was evaluated using regression analysis and comparison between predicted and experimental values. In addition to the overall dataset assessment, the model was further validated on three representative steel grades to examine its practical predictive capability. The corresponding regression plots are presented in Figs. 6 and 7, while the predicted and experimental yield strength values are summarized in Table 4.

The obtained correlation coefficients were $R = 0.835$ for the training dataset, $R = 0.829$ for the validation dataset, $R = 0.864$ for the testing dataset, and $R = 0.833$ for the complete dataset. These results indicate a strong correlation between predicted and experimental yield strength values, confirming that the ANN successfully captured the relationship between chemical composition and yield strength.

Compared to the fatigue strength prediction model, the yield strength ANN exhibits slightly lower data dispersion and a more stable regression trend, which is consistent with the lower experimental variability typically associated with yield strength measurements. The close R values obtained for the training and testing subsets further indicate stable generalization behavior without evidence of overfitting.

Additional validation was performed by comparing ANN-predicted yield strength values with experimentally measured data for three representative steel grades: S355J2 + N, S690QL, and X37CrMoV5-1. The chemical compositions of these steels were used as input data, and the predicted yield strength values were compared with experimental results reported in [13,14]. Comparison is displayed on Fig. 8.

The comparison between predicted and experimental yield strength values shows a good level of agreement for all analyzed steel grades. The average absolute deviation between predicted and experimental values was approximately 37 MPa, corresponding to a mean absolute percentage error (MAPE) of 3.97%. In all three cases, the ANN predictions slightly underestimated the experimental yield strength values, with deviations below 6%.

4. Discussion

The results demonstrate that both developed ANN models achieved stable predictive performance across a wide range of steel grades when chemical composition was used as the sole input. The obtained correlation levels and error magnitudes indicate that the networks successfully learned nonlinear relationships between alloying elements and mechanical properties, despite the heterogeneity of the dataset and the absence of explicit processing and microstructural descriptors.

A comparison between the two models reveals that yield strength prediction exhibits lower scatter and more stable regression behavior than fatigue strength prediction. This behavior is consistent with fundamental differences in the physical nature of these properties. Experimental studies on Cr–Mo steels have demonstrated pronounced scatter in fatigue strength due to microstructural heterogeneity, residual stresses, and testing conditions, supporting the observed variability in fatigue-related predictions [14]. Yield strength is primarily governed by chemical composition and typical strengthening mechanisms associated with alloying and processing routes, whereas fatigue strength is additionally influenced by microstructural imperfections, residual stresses, surface condition, and defect population, which are not explicitly represented in the current dataset. As a result, higher variability and slightly reduced correlation levels are expected for fatigue-related predictions.

The observed systematic deviations—slight overestimation for fatigue strength and slight underestimation for yield strength—suggest that the ANN models captured dominant compositional trends while remaining sensitive to dataset balance and coverage. These systematic trends indicate that the learning process is not random, but rather reflects physically meaningful correlations between alloying elements and mechanical response. In this context, chemical composition acts as a surrogate descriptor for the underlying processing–structure–property relationship, implicitly embedding information related to typical heat-treatment routes and resulting microstructures associated with different steel grades.

From a modeling perspective, the application of Bayesian regularization played a key role in controlling model complexity and ensuring stable generalization behavior. This aspect is particularly important given the relatively high dimensionality of the input space compared to the available number of samples. The consistency between training, validation, and testing results indicates that the networks avoided overfitting and retained predictive capability beyond the training dataset.

Although the ANN models operate as data-driven predictors, the systematic nature of the trends and deviations suggests that the networks learned physically relevant relationships rather than purely numerical correlations. Nevertheless, the absence of explicit descriptors related to microstructure and processing conditions inherently limits the achievable prediction accuracy, particularly for fatigue-related properties. This limitation defines the scope of applicability of the proposed models, which are best suited for preliminary material screening and comparative assessment rather than final design validation.

5. Conclusion

This study demonstrated the applicability of Artificial Neural Networks (ANNs) for predicting key mechanical properties of steels—fatigue strength and yield strength—using chemical composition as the sole input. Based on the presented results, the following conclusions can be drawn:

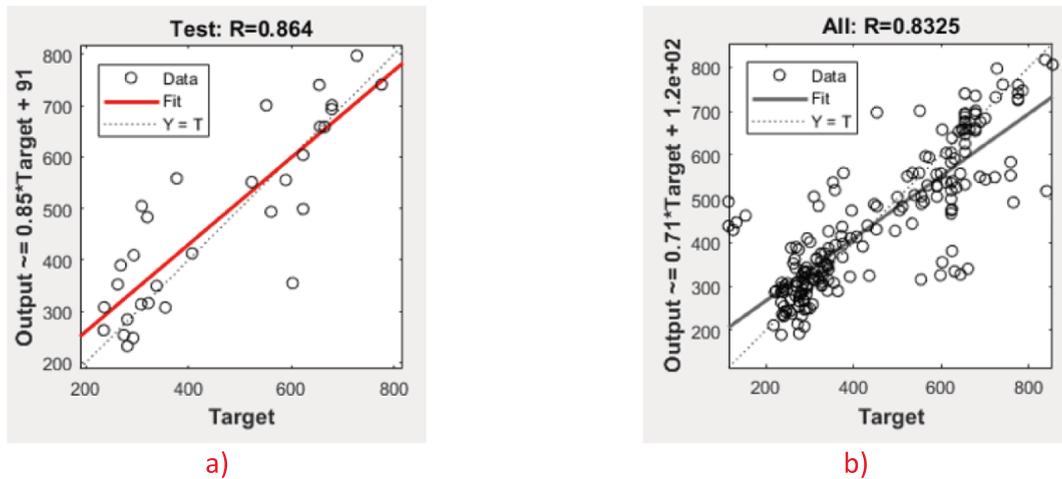


Fig. 7. A) comparison between predicted and experimental yield strength values obtained by the ann model for the testing dataset. b) comparison between predicted and experimental yield strength values obtained by the ann model for the complete dataset.

Table 4
Display of estimated and experimental values of yield strength [14].

Steel grade	S355J2 + N	S690QL	X37CrMoV5-1
Estimated value	391.32	725.54	1440.22
Experimental value	401.24	767.97	1499
Error value, MPa	9.92	42.43	58.78
Error value, %	2.47	5.52	3.9

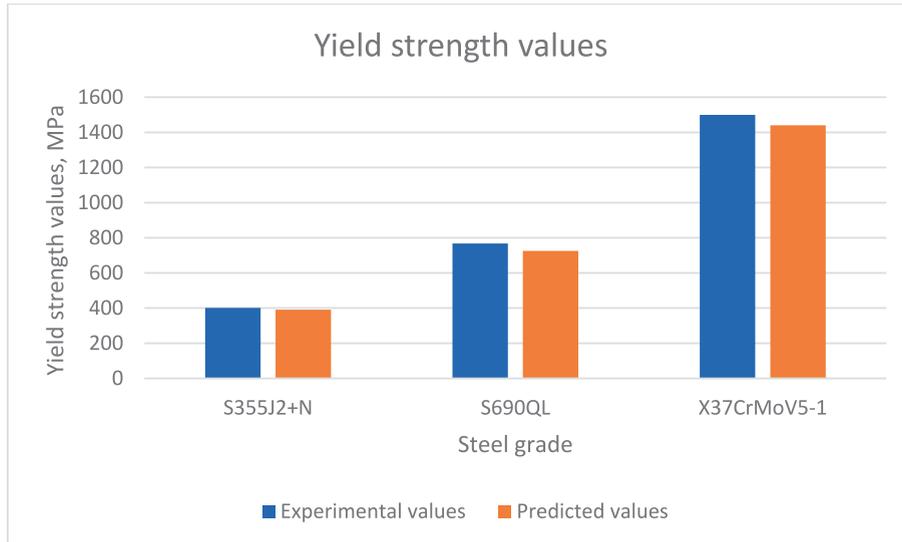


Fig. 8. Graphical interpretation of estimated and experimental values of yield strength.

- (1) Two independent ANN models were successfully developed to predict fatigue strength and yield strength across a wide range of steel grades, including structural, high-strength, and tool steels.
- (2) Both models exhibited stable predictive performance, with correlation coefficients in the range $R = 0.83\text{--}0.90$ and mean absolute percentage errors below 10%, indicating good generalization capability despite the heterogeneous dataset.
- (3) The fatigue strength model showed slightly higher scatter and a small positive bias, whereas the yield strength model demonstrated lower variability and higher stability, reflecting fundamental differences in experimental scatter between fatigue-related and static mechanical properties.

- (4) Validation using three representative steels (S355J2 + N, S690QL, and X37CrMoV5-1) confirmed the ability of both ANN models to provide reliable property estimates, with deviations between predicted and experimental values remaining within acceptable engineering margins.
- (5) The application of Bayesian regularization effectively controlled model complexity and prevented overfitting, ensuring consistent performance across training, validation, and testing subsets even with a limited dataset size.
- (6) The proposed ANN-based framework is suitable for preliminary material screening and comparative property assessment in the early stages of alloy design, where rapid estimation of mechanical properties is required prior to detailed experimental validation.

Future work will focus on expanding the dataset and incorporating additional descriptors related to heat-treatment conditions and microstructural characteristics, as well as exploring hybrid and ensemble modeling strategies to further improve prediction robustness and accuracy.

CRedit authorship contribution statement

Dj. Ivković: Software, Conceptualization. **D. Arsić:** Writing – review & editing, Methodology, Formal analysis. **D. Adamović:** Writing – review & editing, Visualization, Validation, Supervision, Project administration, Investigation, Conceptualization. **A. Sedmak:** Resources, Methodology. **M. Delić:** Software, Data curation, Conceptualization. **R. Vulović:** Writing – review & editing, Validation, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

Data will be made available on request.

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