Machine learning-based prediction of alloying element effects on irradiation swelling in austenitic steels

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Abstract

Austenitic stainless steels have been extensively utilized as key structural components in nuclear reactors, yet they exhibit a strong tendency to undergo swelling under neutron irradiation, which consequently deteriorates their mechanical performance. Hence, reliable prediction of the swelling evolution in austenitic stainless steels is essential to guarantee their operational integrity during reactor service. This research draws on a curated dataset documenting neutron irradiation-induced swelling in austenitic stainless steels, in which correlation analysis and recursive feature elimination were used to identify critical factors governing swelling behavior—namely, temperature, neutron flux, and the concentrations of Cr, Mn, Ni, Si, P, and C. Based on the 15 selected features, a multilayer perceptron (MLP) model was developed for predictive analysis of swelling, enabling precise prediction of the peak swelling temperature and the dose corresponding to the swelling incubation stage. Using the trained MLP model, a quantitative relationship was established between the swelling rate and the elemental concentrations of Cr, Mn, Ni, Si, P, and C. The analysis revealed that higher Cr content consistently promotes swelling, while increases in Si and P (above 0.02 wt.%) effectively suppress swelling. Additionally, there exist threshold concentrations for Mn (2.5 wt.%), Ni (35 wt.%), and C (0.1 wt.%), beyond which swelling is most effectively mitigated. The results of elemental interaction analysis indicate that in austenitic stainless steels containing high levels of Cr, Ni must be increased to 15–20 wt.% to achieve enhanced swelling resistance. Under conditions of low C concentration, increasing the P content appropriately can enhance the material's resistance to irradiation-induced swelling. These findings offer quantitative guidance for designing and optimizing the composition of austenitic stainless steels with improved swelling resistance under irradiation.

Full Text

Preamble

Machine learning-based prediction of alloying element effects on irradiation swelling in austenitic steels*

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Austenitic stainless steels have been extensively utilized as key structural components in nuclear reactors, yet they exhibit a strong tendency to undergo swelling under neutron irradiation, which consequently deteriorates their mechanical performance. Hence, reliable prediction of the swelling evolution in austenitic stainless steels is essential to guarantee their operational integrity during reactor service. This research draws on a curated dataset documenting neutron irradiation-induced swelling in austenitic stainless steels, in which correlation analysis and recursive feature elimination were used to identify critical factors governing swelling behavior—namely, temperature, neutron flux, and the concentrations of Cr, Mn, Ni, Si, P, and C. Based on the 15 selected features, a multilayer perceptron (MLP) model was developed for predictive analysis of swelling, enabling precise prediction of the peak swelling temperature and the dose corresponding to the swelling incubation stage. Using the trained MLP model, a quantitative relationship was established between the swelling rate and the elemental concentrations of Cr, Mn, Ni, Si, P, and C. The analysis revealed that higher Cr content consistently promotes swelling, while increases in Si and P (above 0.02 wt.%) effectively suppress swelling. Additionally, there exist threshold concentrations for Mn (2.5 wt.%), Ni (35 wt.%), and C (0.1 wt.%), beyond which swelling is most effectively mitigated. The results of elemental interaction analysis indicate that in austenitic stainless steels containing high levels of Cr, Ni must be increased to 15–20 wt.% to achieve enhanced swelling resistance. Under conditions of low C concentration, increasing the P content appropriately can enhance the material's resistance to irradiation-induced swelling. These findings offer quantitative guidance for designing and optimizing the composition of austenitic stainless steels with improved swelling resistance under irradiation.

Keywords: Austenitic stainless steel, Void swelling, Machine learning, Alloying elements, Irradiation

Introduction

Owing to their outstanding mechanical strength and corrosion resistance, austenitic stainless steels have been extensively employed as structural components in light water reactor systems, and are regarded as promising candidates for fuel cladding in Generation IV fast neutron reactors [**?**]. Nevertheless, austenitic stainless steels are particularly vulnerable to swelling under irradiation, due to the irradiation-induced generation of dense cavities, voids, and dislocation loops, which cause substantial volumetric expansion, thereby degrading the mechanical integrity of the material. As reported by Garner, an irradiation swelling rate as high as 86.36% was observed in 20% cold-worked 316 austenitic stainless steel following exposure to a fast neutron fluence of 27.16×10^{22} n/cm^2 at 510 °C [?]. The swelling behavior of austenitic stainless steels under irradiation is governed by complex interactions among alloying elements, thermomechanical processing, and irradiation environment, which has hindered a comprehensive understanding of the swelling mechanisms, thereby posing substantial challenges to the accurate prediction of swelling trends in austenitic stainless steels.

At present, only a limited number of irradiation swelling prediction models for austenitic stainless steels have been publicly reported, among which Kalchenko [?] developed an empirical model for predicting the swelling behavior of 18Cr10NiTi austenitic stainless steel, but this model was constructed using a limited experimental dataset, and its applicability and accuracy require further validation. In addition, most current swelling models emphasize the prediction of the linear swelling stage, characterized by a swelling rate that levels off at approximately 1% per dpa beyond a critical neutron fluence, whereas the accurate estimation of the incubation dose remains insufficiently addressed. In addition to the incubation dose and peak temperature, which are critical for predicting irradiation swelling trends, the addition of alloying elements enables precise tailoring of swelling resistance in austenitic stainless steels.

For Fe–Cr–Ni austenitic stainless steels, studies [?] demonstrate that under fixed irradiation temperature and flux conditions, chromium content exhibits a monotonic influence on swelling, where swelling magnitude progressively increases with elevated chromium content. Nevertheless, nickel content exhibits threshold behavior in its influence on irradiation swelling. As nickel content increases, swelling magnitude first undergoes rapid decline, reaching a minimum value at a specific nickel concentration. Beyond this point, swelling gradually increases at a moderate pace. Consequently, reducing chromium content while increasing nickel concentration enhances irradiation swelling resistance in austenitic stainless steels. Further optimization involves tailoring minor alloying elements (e.g., C, Ti, Si, P, Nb, V, B, Mn, N), leading to the development of next-generation cladding materials through this compositional design strategy. Representative alloys include Japan's PNC316, France's 15-15Ti, and America's D9 [?]. These minor alloying additions demonstrate pronounced influences on swelling behavior [?, ?, ?, ?], with four principal suppression mechanisms: (1) Enhanced vacancy diffusion coefficients reduce vacancy supersaturation, inhibiting void/cavity nucleation and growth (e.g., Si, P, Ti); (2) Coherent carbide precipitates (TiC, NbC, VC) formed through reactions of titanium, niobium, or vanadium with carbon serve as defect sinks for vacancies; (3) γ-phase stabilization via carbon, nitrogen, and manganese additions suppresses $M_{23}C_6$ and Ni_3Si precipitation, preventing matrix depletion of nickel, silicon, or titanium and consequent swelling acceleration; (4) Boride/phosphide precipitates pin dislocations, absorbing vacancies and transmutation helium to achieve swelling suppression.

Given the complex interdependencies between alloying elements and irradiation swelling in austenitic steels, current alloy design relies predominantly on empirical compositional tuning. This approach is constrained by the resource-intensive nature of irradiation experiments, where substantial costs, protracted timelines, and environmental specificities restrict holistic evaluation of elemental interactions and their collective impact on swelling phenomena. At the microscopic level, alloying elements engage in complex interactions with irradiation-induced defects. Multiscale computational modeling provides critical insights into swelling mechanisms, where the methodology seeks to track defect evolution across spatiotemporal scales while capturing the complete lifecycle of defect generation, diffusion, annihilation, and aggregation. This approach enables prediction of material swelling behavior through simulations of void, dislocation loop, and helium bubble distributions [?, ?]. Nevertheless, the multiscale nature of irradiation damage (atomic defects $\rightarrow$ macroscopic swelling) necessitates experimental calibration of critical model parameters, especially for gas atom dynamics [?] and minor alloying element roles [?]. Such reliance inherently limits precise quantitative prediction of swelling evolution.

In recent years, machine learning approaches have gained significant attention for materials composition design and performance prediction, owing to their robust capability for multidimensional nonlinear mapping, which enables extraction of hidden patterns from complex datasets [?]. Machine learning methods establish complex nonlinear correlations between input features (e.g., composition, heat treatment parameters) and output properties (e.g., tensile strength, yield strength) based on mathematical statistics principles, thereby enabling efficient prediction of material performance. Kemp et al. [?] employed artificial neural networks to investigate the effects of material composition, testing temperature, and irradiation parameters on the yield strength of 9Cr steels, revealing that testing temperature and irradiation temperature exert the most pronounced influence, while increased nickel content also contributes to a marked enhancement in yield strength. Jin et al. [?] implemented machine learning to predict the onset of irradiation swelling in nuclear structural materials, including austenitic stainless steels and ferritic-martensitic steels, based on an established experimental dataset. Machine learning algorithms have also seen increasing application in predicting hardening and embrittlement trends of reactor pressure vessels (RPVs) [?, ?, ?]. Based on surveillance data from international and Chinese domestic reactor pressure vessel steels, Chu et al. developed a simplified fluence-dependent model to predict transition temperature shift [?]. Ferreño et al. employed machine learning algorithms, including gradient boosting trees and neural networks, to investigate variables influencing irradiation embrittlement ($\Delta T_{41}J$) in reactor pressure vessel steels. Their analysis identified unirradiated yield strength (YS(u)) as a newly significant predictor alongside nickel content and irradiation temperature, enhancing model accuracy with a 7% reduction in root mean square error (RMSE) and a 15% increase in the coefficient of determination (R^2) [?]. In addition, artificial neural networks can effectively investigate key factors influencing the creep lifetime of oxide dispersion-strengthened (ODS) steels [?]. Machine learning algorithms thus represent an essential tool for forecasting mechanical performance and critical determinants in key reactor materials. Their application to irradiation swelling phenomena in austenitic stainless steels promises substantial scientific value.

This study compiles irradiation swelling data for austenitic stainless steels from published literature. Based on this dataset, six supervised machine learning models are trained, while feature selection identifies key variables for predicting swelling magnitude. Building on the optimized dataset comprising 15 feature variables, this work constructs a multilayer perceptron (MLP) model. This model predicts irradiation swelling magnitude in austenitic stainless steels, while quantitatively analyzing relationships between swelling magnitude and six key alloying elements (Cr, Mn, Ni, Si, P, C). The analysis further decouples synergistic effects among these elements, ultimately predicting optimal compositional ranges that minimize swelling magnitude. These findings enable accurate forecasting of irradiation swelling behavior, offering strategic insights for alloy design to improve irradiation swelling resistance in austenitic stainless steels.

2.1. Data Collection and Curation

The dataset used in this study is derived from experimental results reported in the literature and technical reports [?, ?, ?, ?, ?, ?, ?, ?, ?]. It includes the chemical compositions of alloying elements in austenitic stainless steels, intrinsic dislocation density, irradiation parameters (pre-irradiation fluence, total neutron fluence, and irradiation temperature), as well as the corresponding irradiation-induced swelling rate data. Notably, several experiments incorporated pre-irradiation treatment with the aim of introducing microstructural defect sinks prior to the main irradiation. This approach was intended to suppress vacancy clustering and void formation during subsequent high-dose exposure, thereby delaying or mitigating irradiation-induced swelling. In addition, given that the processing history exerts a significant influence on the irradiation swelling behavior of austenitic stainless steels, this study uses intrinsic dislocation density as a surrogate parameter to represent this effect. The dislocation density can be estimated using a modified Rietveld refinement method [?]. For example, 20% cold-worked 316 stainless steel typically exhibits a dislocation density of approximately 3.6×10^{15} m^{-2}.

The austenitic stainless steel irradiation swelling dataset established in this work comprises 668 individual samples, each consisting of 23 feature variables (e.g., elemental composition, intrinsic dislocation density, and irradiation parameters) and a single target variable, i.e., irradiation swelling rate, all expressed as numerical values. In order to gain insight into the numerical distribution of each feature variable, the minimum, maximum, and average values were computed for all features, as presented in Table 1 . The target variable (irradiation swelling magnitude) in the dataset is presented in Fig. 1 [Figure 1: see original paper]. Swelling magnitude values exhibit a broad distribution range (−10% to 90%), resulting from variations in irradiation conditions, material compositions, and characterization methodologies. For example, under identical irradiation conditions, solution-annealed and 20% cold-worked austenitic stainless steels exhibit contrasting swelling responses: the cold-worked variant demonstrates negative swelling magnitude. The dataset reveals a non-uniform swelling distribution, with the predominant range (60% of data) at 0–10%, followed by 10–20% (12%) and 20–30% (7%) swelling magnitude intervals, with the remainder distributed across other ranges.

Table 1. The summary for each feature in the dataset.

Features	Description	Minimum	Maximum	Average
Temperature (°C)				
Pre-Φ	Pre-irradiation fluence (10^{22} n/cm^2)			
Φ	Irradiation fluence (10^{22} n/cm^2)			
Dislocation density (10^{14}/m^2)				
Fe fraction (wt.%)				
Cr fraction (wt.%)				
Ni fraction (wt.%)				
Mo fraction (wt.%)				
Mn fraction (wt.%)				
Si fraction (wt.%)				
C fraction (wt.%)				
Al fraction (wt.%)				
B fraction (wt.%)				
Co fraction (wt.%)				
Nb fraction (wt.%)				
Cu fraction (wt.%)				
N fraction (wt.%)				
P fraction (wt.%)				
S fraction (wt.%)				
Ta fraction (wt.%)				
Ti fraction (wt.%)				
O fraction (wt.%)				
Pb fraction (wt.%)				

Notably, the measurement methods used for the samples in Table 1 differ among sources, resulting in variability in the quality and accuracy of the data. In addition, the dataset integrates physically distinct characteristics with heterogeneous units (e.g., elemental concentrations, dislocation density, irradiation flux). Specimens derived from divergent experimental protocols and material processing histories further exacerbate feature-scale disparities. These magnitude variations spanning multiple orders may induce gradient instabilities during model optimization, consequently diminishing convergence efficiency and prediction fidelity, necessitating feature scaling methodologies. Consequently, prior to model training, this work applies Z-score normalization to all feature data [?], as formalized in Eq. (1).

$$z = \frac{x - \mu}{\sigma}$$

where z denotes the standardized data, x is the original value, μ is the mean, and σ is the standard deviation of the corresponding feature, all calculated from the training set. As prescribed by Eq. (1), each feature is transformed to zero mean and unit variance, scaling the variables listed in Table 1 predominantly within the range of $[-1, 1]$. This normalization procedure effectively eliminates dimensional heterogeneity and magnitude disparities that could otherwise compromise prediction fidelity.

2.2. Machine Learning Models

Machine learning algorithms are broadly classified into supervised and unsupervised types. Given that the irradiation swelling dataset used in this study has clearly defined targets and exhibits nonlinear relationships in a high-dimensional feature space, six supervised machine learning models were employed for training. These include Decision Tree Regression (DTR) [?], Random Forest (RF) [?], Support Vector Regression (SVR) [?, ?], Gradient Boosting Regression (GBR) [?], K-Nearest Neighbors (KNN) [?], and Multilayer Perceptron (MLP) [?]. To evaluate the generalization ability and predictive accuracy of the machine learning models, both the hold-out method and cross-validation were employed. In the hold-out approach, 80% of the entire dataset was used for model training, while the remaining 20% was reserved for testing the predictive performance of the trained models.

The fitting performance of the machine learning models was evaluated using the coefficient of determination (R^2) and the root mean square error (RMSE), as defined in Eq. (2) and Eq. (3).

$$R^2 = 1 - \frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2}$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{n}}$$

where n is the number of samples; y_i and $\hat{y}_i$ represent the experimental and predicted values of the i-th sample ($i = 1, 2, ..., n$); and $\bar{y}$ denotes the mean of the experimental values.

Cross-validation was employed to determine the optimal values of the model's hyperparameters, as these tunable parameters have a substantial impact on predictive performance. In this study, k-fold cross-validation was employed by partitioning the training dataset into k equally sized folds. One fold was used for validation, while the remaining $k-1$ folds were used to train the model. In this way, for a given set of hyperparameters, the model is evaluated k times, and the average predictive performance across the k folds is taken as the final evaluation metric. Critically, initial parameter space definition requires assignment of plausible value ranges to each hyperparameter. Subsequently, the grid search technique is employed to systematically generate the complete set of possible parameter combinations, enabling comprehensive model optimization. Following comprehensive evaluation of all parameter combinations, their predictive performances are comparatively assessed. The configuration yielding the highest cross-validated performance metric is designated as optimal. This methodology maximizes information extraction from limited sample data while preventing overestimation artifacts induced by stochastic dataset partitioning.

Notably, k-fold cross-validation enables rigorous determination of optimal tunable parameters for any specific training dataset, concurrently mitigating overfitting risks while maximizing generalization capability. However, divergent training datasets may yield distinct optimal parameter combinations, introducing selection inconsistency. To mitigate this variability, the complete dataset undergoes 100 independent partitioning iterations, generating 100 unique training subsets. Each subset determines an optimal parameter combination via cross-validation. The most frequently occurring combination is then designated as the final tunable parameter set, effectively circumventing misleading optimization artifacts induced by sampling stochasticity. Table 2 lists the optimal values for parameters in six machine learning models.

Table 2. Optimal values for parameters in six ML models.

Model	Optimal hyperparameters
GBR	learning_{rate}=0.08, max_{depth}=4, max_{features}=sqrt, n_{estimators}=1600
MLP	activation=relu, alpha=0.0001, hidden_{{{layer}}{{sizes}}}=(64, 32, 16), learning{rate}=constant, solver=adam
RFR	max_{depth}=17, max_{features}=sqrt, min_{{{samples}}{{leaf}}}=1, min{{{samples}}{{split}}}=2, n{estimators}=300
SVR	C=1000, epsilon=1, gamma=auto, kernel=rbf
DTR	max_{depth}=7, max_{features}=None, splitter=random
KNN	n_{neighbors}=17, weights=uniform

2.3. Feature Selection

The absence of redundancy evaluation for the 23 experimental features (Table 1) necessitates systematic feature selection, enabling identification of key feature combinations for irradiation swelling prediction models. Inter-feature Pearson correlation coefficients (PCC) were computed per Eq. (4) to evaluate variable dependencies.

$$\rho(u,v) = \frac{(u-\bar{u})^T(v-\bar{v})}{\sqrt{(u-\bar{u})^T(u-\bar{u})\cdot(v-\bar{v})^T(v-\bar{v})}}$$

where u and v represent feature columns, and $\bar{u}$ and $\bar{v}$ represent their mean values.

The PCC ranges from -1 to 1, where positive values indicate a positive correlation between two features, and negative values indicate a negative correlation. Absolute values exceeding 0.9 ($|\rho| > 0.9$) indicate feature redundancy requiring removal to constrain model complexity and suppress overfitting. By selectively eliminating one feature from each redundant pair to generate two derivative subsets, identical machine learning models are trained and tested on both modified datasets. Retention decisions are based on comparative analysis of test set prediction errors (RMSE), preserving features from the subset minimizing error degradation. This strategy ensures preferential retention of features exerting significant impacts on model accuracy. Subsequent refinement employs recursive feature elimination (RFE), an iterative selection methodology that sequentially removes minimally influential features through repeated model training and importance ranking. Implementation requires cyclical calculation of feature significance scores, subsequent ranking of variables, and systematic pruning of minimally contributive features during each iteration cycle, per the schematic in Fig. 2 [Figure 2: see original paper].

Fig. 2. Workflow schematic of recursive feature elimination (RFE).

3.1. Model Prediction

Six machine learning models (DTR, RFR, SVR, GBR, KNN, and MLP) were trained and tested 100 times using the normalized dataset. The average RMSE and R^2 values obtained on the test sets are presented in Fig. 3 [Figure 3: see original paper]. A lower RMSE (closer to 0) and a higher R^2 (closer to 1) indicate better model fitting performance. As shown in Fig. 3, among the six evaluated models, the MLP model achieved the lowest RMSE (2.978%) and the highest average R^2 (0.93) on the test set, indicating its superior accuracy in fitting the collected irradiation swelling data of austenitic stainless steels. Accordingly, the MLP model was selected for subsequent predictive analyses of the relationships among alloy composition, temperature, irradiation dose, and swelling rate.

Fig. 3. RMSE and R^2 values of various machine learning models used to predict irradiation swelling.

For machine learning models designed to predict material properties, their predictive performance heavily depends on the selected features. However, at this stage, redundancy among input variables has not been considered, and key features influencing swelling behavior remain to be identified. Therefore, it is necessary to perform feature selection in the subsequent step to eliminate redundancy and identify the most informative variables. Fig. 4a [Figure 4: see original paper] presents the correlation heatmap of the 23 feature variables listed in Table 1. Except for Ta and Pb, whose Pearson correlation coefficient (PCC) has an absolute value of 1, all other feature pairs exhibit absolute PCCs ≤ 0.90, indicating that most features do not exhibit significant redundancy. However, the perfect linear correlation between Ta and Pb implies duplicated information, which may affect model stability and predictive accuracy. Therefore, redundant features must be addressed prior to model training. Retaining all other feature variables in the dataset, two separate models were trained after individually removing either Ta or Pb. As shown in Fig. 4b, the dataset with Ta removed yielded a lower RMSE (2.988%), indicating better predictive performance. Consequently, Pb was retained and Ta was excluded from the dataset for subsequent model application.

Fig. 4. (a) Heatmap of the correlations among the 23 feature variables; (b) Prediction results based on datasets with Ta or Pb removed individually.

Application of the Fig. 2 RFE framework initiated with feature significance ranking in the Ta-depleted dataset. Systematic elimination proceeded through ascending-ordered removal of minimally influential features. Corresponding MLP training and RMSE-based prediction validation were executed post-pruning. Fig. 5 [Figure 5: see original paper] quantifies MLP prediction RMSE evolution during feature reduction. The marginal oscillations observed during sequential removal of least contributive features substantiate their limited effect on irradiation swelling rate modeling. After reduction to fewer than five features, RMSE undergoes substantial deterioration. This evidences the necessity of feature ensembles, where dominant variables cooperatively interact with moderately significant counterparts through nonlinear coupling effects, a fundamental mechanism in irradiation swelling prognostication. Irradiation swelling evolves through multiphysics-activated cooperations across multidimensional features. When feature space dimensionality falls below critical thresholds, models fail to resolve essential interactive dependencies, directly impairing swelling prediction accuracy. Across the feature dimensionality range of 5 to 22 variables, RMSE values exhibit remarkable stability (2.84%–3.34%), with optimal predictive performance achieved at the 15-feature configuration, as marked by the asterisk in Fig. 5. This irradiation-optimal feature subset comprises temperature (Temp), neutron flux (Φ), intrinsic dislocation density ( ), and composition of 12 alloying elements categorized by nuclear significance: chromium, iron, and nickel as matrix constituents; manganese, silicon, titanium, and molybdenum as micro-alloying agents; carbon and oxygen as interstitial elements; phosphorus and sulfur as grain-boundary segregation controllers; along with boron as the neutron-absorbing species.

Fig. 5. Evolution of RMSE versus feature count during recursive feature elimination (RFE) selection.

3.2. Predictive Accuracy of the MLP Model

Utilizing these 15 optimally selected features, the MLP model demonstrates high-fidelity prediction of irradiation swelling rates, as validated in Fig. 6 [Figure 6: see original paper]. The model exhibits robust predictive capability on both training and test datasets, achieving RMSE values of 2.67% and 2.79%, alongside R^2 coefficients of 0.98 and 0.97, respectively. These metrics indicate exceptional agreement between predicted and experimental swelling rates. Furthermore, the majority of data points cluster tightly along the unity-slope line (where predicted swelling equals measured values), confirming the model's superior accuracy while substantiating that these 15 features comprehensively characterize irradiation swelling behavior in austenitic stainless steels.

Fig. 6. MLP model prediction accuracy for irradiation swelling using key feature inputs.

To further validate the generalization capability of the trained MLP model for irradiation swelling prediction, an independent experimental dataset withheld from model training was employed for verification. Comparative analysis between experimentally measured swelling rates [**?**, **?**] and model predictions, as presented in Fig. 7 [Figure 7: see original paper], demonstrates robust extrapolation performance across diverse irradiation conditions. Overall, predicted irradiation swelling values demonstrate close alignment with experimental measurements for both AISI 316 and X15893 austenitic stainless steels, with particularly excellent agreement for AISI 316. Relatively significant deviations occur between predictions and measurements for X15893, attributable to compounded factors amplifying prediction complexity. Crucially, the presence of 0.3 wt.% Cu and Co in X15893 alloy—elements omitted from the model's feature space—prevents the MLP from learning their underlying influence mechanisms on swelling behavior. Existing studies [**?**, **?**] demonstrate that Cu nonlinearly modulates irradiation swelling through mechanisms including enhanced second-phase precipitation and regulation of point defect migration/clustering. Co primarily influences swelling by reducing stacking fault energy (SFE) to stabilize austenitic phase structure and suppress deformation-induced martensitic transformation, thereby delaying detrimental microstructural evolution [**?**, **?**]. Furthermore, as irradiation swelling constitutes a multiphysics-driven complex response, its evolution inherently involves synergistic couplings among multiple alloying elements and processing parameters. The exclusion of Cu and Co from model training prevents recognition of their direct effects on target variables while hindering capture of potential interactions with other input variables, consequently inducing prediction biases for specialty alloys like X15893.

Fig. 7. Comparison between MLP-predicted and experimentally measured irradiation swelling rates in independent validation datasets.

Interpretability Analysis of Irradiation Swelling Prediction Models

As noted above, fifteen feature variables, namely temperature (Temp), neutron flux (Φ), intrinsic dislocation density ( ), and the contents of Ni, Fe, Si, O, Mo, B, S, Ti, C, P, Mn, and Cr, were found to be closely associated with the swelling behavior of neutron-irradiated austenitic stainless steel. To further investigate how these key features influence the swelling rate, Shapley Additive exPlanations (SHAP) [**?**] were employed to interpret the predictive model. SHAP interprets the model output as a cooperative game payout, in which each feature's contribution is assessed by averaging its marginal impact across all possible feature combinations, thereby quantifying its importance in driving the model's prediction. It is important to note that the SHAP values are computed based on a specific data split, and as such, the resulting feature importance is highly dependent on how the training dataset is partitioned. To validate the robustness of the identified feature rankings and mitigate potential bias introduced by favorable data splits, the dataset was randomly divided into training and testing sets using 50 different splitting schemes. The distribution of the absolute mean SHAP values of 15 selected features, averaged over 50 repeated training runs, is presented in Fig. 8 [Figure 8: see original paper]. Features with larger absolute SHAP values are considered to exert a greater influence on the final predictions, while those with smaller values are regarded as having minimal impact. From the results, neutron flux (Φ) and irradiation temperature (Temp) are identified as the most influential factors affecting the swelling rate of austenitic stainless steel under neutron irradiation. In terms of alloy composition, Cr, Mn, Ni, Si, P, and C were found to have significant impacts on the irradiation-induced swelling of austenitic stainless steel, particularly the three primary alloying elements: Cr, Mn, and Ni. Although Fe also exhibited relatively high SHAP values, it was excluded from further consideration since it serves as the matrix element. Therefore, only the effects of additional alloying elements were considered, with the aim of providing guidance for improving swelling resistance from the perspective of compositional design.

Fig. 8. Significance hierarchy of critical features governing irradiation swelling predictions in neutron-irradiated austenitic stainless steels.

4.1. Effect of Temperature and Dose

Section 3.3 presents the results of the feature importance analysis, which identify Φ and Temp as the most influential factors affecting irradiation swelling in austenitic stainless steels. Based on this finding, the MLP model was used to predict the variation of swelling rate with respect to these two variables. The predicted trends are shown in Fig. 9 [Figure 9: see original paper]. As illustrated in Fig. 9a, the MLP model accurately captures the non-monotonic dependence of swelling rate on temperature, with the maximum swelling occurring at 463 °C. This value falls within the experimentally reported range of 445 to 520 °C [?], confirming the model's reliability. Fig. 9b shows that the swelling rate remains nearly zero at low neutron fluence and begins to increase rapidly after a certain threshold is reached. This behavior suggests two distinct stages of swelling: an initial incubation period followed by a swelling growth phase. The predicted irradiation doses marking the transition from incubation to rapid swelling are 88 dpa at 400 °C, 37.85 dpa at 525 °C, and 73 dpa at 600 °C. These predictions are in good agreement with experimental data, including the incubation dose of 36 dpa reported by Bruce J. Makenas [?] at 513 °C. At intermediate temperatures (525 °C), swelling initiates rapidly at lower doses and reaches peak rates due to optimal defect dynamics. In contrast, low temperatures extend incubation periods by restricting defect diffusion and clustering, while high temperatures suppress swelling through enhanced vacancy-interstitial recombination that inhibits void nucleation.

Fig. 9. MLP-predicted irradiation swelling rate evolution (a) versus irradiation temperature, (b) versus neutron flux.

4.2. Effect of Alloying Elements

Based on feature importance analysis (Fig. 8), Cr, Mn, Ni, Si, P, and C are identified as pivotal alloying elements governing irradiation swelling rates in austenitic stainless steels. To further investigate the influence of these six elements on swelling behavior, single-factor sensitivity analysis was conducted using the optimized MLP model. When predicting a target element's impact (e.g., Mn, Si, P, or C), the Fe–Cr–Ni ternary alloy system served as the baseline with Cr and Ni concentrations fixed at representative mean values from the training dataset, while varying the target element's content and maintaining Fe balance. For Cr and Ni sensitivity assessments, predictions were performed by varying one element's concentration range while fixing the other. Concentrations of all non-essential elements listed in Table 1 were rigorously set to 0 wt.%, preserving only the six key elements and matrix Fe. This purification protocol creates an isolated evaluation environment where swelling responses can be unambiguously attributed to individual elemental variations.

Under neutron irradiation at 8.6×10^{22} n/cm^2 and 525°C, the MLP model mapped irradiation swelling responses of Fe–Cr–Ni austenitic steels to controlled variations in Cr, Ni, Si, P, and C concentrations, revealing element-specific swelling thresholds shown in Fig. 10 [Figure 10: see original paper]. The analysis reveals a monotonic positive correlation between Cr content and irradiation swelling rate in Fe–Cr–Ni austenitic stainless steels, where swelling increases progressively with rising Cr concentrations (Fig. 10a). Similarly, swelling exhibits a monotonic inverse relationship with Si content, indicating that controlled Si additions effectively suppress irradiation swelling in these alloys (Fig. 10f). Relevant experimental and theoretical studies [?, ?] have provided mechanistic insights into the role of Si in irradiation-induced swelling behavior. Si is considered a fast-diffusing solute atom that can significantly enhance the effective vacancy diffusion rate in austenitic stainless steels, thereby suppressing vacancy supersaturation and nucleation, which in turn delays cavity formation and the onset of irradiation swelling. Moreover, Si may form neutral complexes with interstitial atoms, indirectly promoting vacancy–interstitial recombination and further reducing the effective defect concentration. Under irradiation, Si tends to segregate at defect sinks such as dislocations and voids, and may co-precipitate with Ni to form Si-rich Ni_3Si (γ) or G-phase particles. These precipitates are capable of increasing the cavity nucleation energy barrier through interfacial trapping mechanisms, thereby substantially extending the swelling incubation period. In addition, some studies [**?**] have suggested that the presence of Si can inhibit helium atom adsorption to a certain extent, increase the migration energy barrier of He atoms, and thus retard helium accumulation and bubble formation.

The effects of Mn, Ni, P, and C contents on the irradiation swelling rate were found to be non-monotonic. As the concentrations of Mn, Ni, and C increased, the swelling rate initially decreased sharply (Fig. 10b, c, e). After reaching a certain critical content, the swelling rate reached a minimum and then began to increase gradually. These results suggest that threshold concentrations exist for Mn, Ni, and C that correspond to the optimal suppression of irradiation-induced swelling, which are approximately 2.5 wt.% for Mn, 35 wt.% for Ni, and 0.1 wt.% for C. Maintaining the concentrations of these elements near their respective thresholds may enhance the swelling resistance of austenitic stainless steels under neutron irradiation. In the case of phosphorus (Fig. 10d), an initial increase in P content leads to a rise in swelling rate, with the peak swelling occurring at approximately 0.02 wt.% P. When the P content exceeds this threshold, the swelling rate of austenitic stainless steel decreases rapidly. Notably, the predicted trends in swelling rate as a function of alloying element content, as shown in Fig. 10, are consistent with previous experimental findings [**?**, **?**], further demonstrating the high predictive accuracy of the MLP model in capturing the irradiation swelling behavior of austenitic stainless steels.

Fig. 10. Predicted relationships between irradiation swelling rate and the concentrations of individual alloying elements: (a) Cr, (b) Mn, (c) Ni, (d) P, (e) C, and (f) Si.

In practice, the effects of alloying elements on irradiation-induced swelling in austenitic stainless steels are governed by coupled and synergistic interactions among the elements themselves. These interactions can be effectively evaluated and analyzed using machine learning algorithms. As shown in Fig. 11a [Figure 11: see original paper], a clear synergistic interaction exists between the two principal alloying elements, Cr and Ni, in influencing the irradiation swelling behavior of austenitic stainless steels. While increasing Cr content leads to higher swelling rates (as observed in Fig. 10a), a simultaneous increase in Ni content significantly mitigates swelling. For instance, as Cr content increases from 10 wt.% to 16 wt.%, the Ni concentration corresponding to the minimum swelling rate also increases from 15 wt.% to 20 wt.%. This indicates that Ni addition is effective in reducing swelling at lower Cr contents and becomes even more critical at higher Cr levels. In other words, increasing Ni content enhances the swelling resistance of austenitic stainless steels, particularly under conditions of elevated Cr concentration. For steels with high Cr content, a concurrent increase in Ni is necessary to effectively suppress irradiation-induced swelling.

In addition to the adverse effect of Cr on irradiation swelling, the addition of P at concentrations below 0.03 wt.% was found to increase the swelling rate. To further investigate the synergistic effect between P and Si, an element known to suppress swelling, their combined influence was analyzed, as shown in Fig. 11b. When the P content exceeds 0.03 wt.%, no significant synergistic interaction is observed between Si and P. Swelling remains low regardless of the amount of Si added, since both elements individually contribute to swelling suppression at higher concentrations. However, when the P content is below 0.03 wt.%, a distinct interaction emerges. As P content increases, the Si concentration corresponding to the minimum swelling rate shifts from 0.2 wt.% to 0.9 wt.%. This indicates that increasing the Si content is necessary to offset the swelling-promoting effect of low-level P additions and improve overall swelling resistance.

In addition, a synergistic interaction exists between trace elements P and C, as illustrated in Fig. 11c. When the P content increases while the C content remains low, the suppressive effect of P on irradiation swelling in austenitic stainless steels becomes more pronounced. As the P content rises from approximately 0.02 wt.% to 0.08 wt.% with the C content kept below about 0.05 wt.%, a significant reduction in the swelling extremum is observed. This indicates that under low C conditions, increasing P effectively mitigates irradiation swelling. Conversely, at higher C levels, where carbon readily promotes carbide formation, the enhancement of swelling suppression by increasing P content becomes even more critical and further improves the material's irradiation resistance.

Fig. 11. Coupling effects of different alloying elements on irradiation swelling rate: (a) Cr–Ni, (b) P–Si, (c) P–C.

5. Conclusion

In this study, approximately 668 irradiation swelling data points of austenitic stainless steels were collected, including irradiation temperature, neutron flux, processing methods, and alloy composition. The dataset was cleaned and filtered before modeling using machine learning techniques. After systematically comparing six commonly used machine learning algorithms, the MLP algorithm was selected to construct the irradiation swelling prediction model. Key feature variables were identified using correlation screening and recursive feature elimination, resulting in a subset comprising Temp, Φ, , and concentrations of twelve alloying elements. The model was further optimized, achieving a final predictive accuracy with $R^2 = 0.97$ and RMSE = 2.79%. Its strong generalization ability was validated by comparing predictions with swelling data from an independent test set. The MLP model was employed to establish the relationship between swelling rate and variables including Temp, Φ, and alloying elements such as Cr, Ni, P, and Si. The following conclusions were drawn:

1. The most important features identified by the MLP model, irradiation temperature and neutron flux, exhibit swelling behavior consistent with established understanding. Specifically, the model predicted a peak irradiation swelling temperature of 463 °C. At a moderate temperature of 525 °C, the predicted incubation dose for irradiation swelling was 37.85 dpa. These predictions agree well with experimentally reported values.

2. The effects of Cr and Si contents on irradiation swelling rate in austenitic stainless steels are monotonic. Cr has an adverse effect on swelling, whereas Si effectively suppresses it. Increasing the contents of Mn, Ni, and C initially reduces the swelling rate but subsequently causes it to rise. Optimal suppression of irradiation swelling is achieved when the concentrations of Mn, Ni, and C reach approximately 2.5 wt.%, 35 wt.%, and 0.1 wt.% respectively. The addition of phosphorus initially promotes swelling, but when its content exceeds 0.02 wt.%, the swelling rate decreases rapidly.

3. Synergistic effects exist among alloying elements. An increase in Cr content promotes irradiation swelling in austenitic stainless steels, while the addition of Ni suppresses this swelling. Furthermore, when P content increases under conditions of low C content, the inhibitory effect of P on irradiation swelling becomes more pronounced.

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