Modeling Void Swelling in 20% Cold-Worked 316 Stainless Steel under Molten Salt Reactor Conditions: A Data-Driven Approach

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1. Introduction

Structural materials in molten salt reactors (MSRs) are subjected to extreme service conditions involving high temperatures, corrosive salt chemistry, and fast neutron irradiation. These environments drive microstructural changes that accumulate over long periods of operation [1]. Among these changes, void swelling is particularly critical because it leads to volumetric expansion, density reduction, and eventual loss of mechanical integrity. The swelling behavior of austenitic stainless steels has been extensively investigated and modeled in the context of fast breeder reactors [2]. In particular, studies on 20% cold-worked AISI 316 stainless steel irradiated in the Experimental Breeder Reactor-II (EBR-II) have demonstrated a transient incubation stage followed by a steady-state swelling rate. Mechanistic models such as rate theory have been developed to predict this behavior [3], but they still struggle to accurately reproduce detailed experimental trends. Although machine learning models have been introduced, their limited generalizability and reduced interpretability hinder broader application [4]. In this study, we propose a data-driven nonlinear modeling approach, aiming to achieve higher predictive accuracy and near-term applicability.

2. Methodology

2.1 Dataset construction

The dataset for this study was compiled from published irradiation experiments on stainless steels in EBR-II. Data were standardized in terms of swelling percentage, irradiation temperature, and dose expressed as displacements per atom (dpa). The original experiments were conducted to minimize specimen-to-specimen scatter, and data from reinserted specimens irradiated at multiple exposures were utilized. This procedure allowed clearer observation of post-transient swelling rates. The resulting dataset encompassed over 44 points across a temperature range of 400–650 °C and doses up to 125 dpa.

2.2 Statistical modeling

Two complementary modeling strategies were applied. First, a polynomial–power law correlation, $\Delta V/V$ (%) = A·(dpa)^n, was used. Second, a logistic-kernel equation that explicitly accounts for the incubation dose and the steady-state swelling rate was employed. Both models are nonlinear and were fitted in R using nonlinear regression.

3. Results and Discussion

The compiled data confirmed that swelling exhibits a strong dependence on temperature. A pronounced swelling peak was observed near 500–550 °C, consistent with enhanced point defect mobility in this regime. Below 450 °C, swelling was suppressed due to limited vacancy migration, whereas above 650 °C, recovery processes reduced void nucleation efficiency. These findings indicate that candidate MSR materials must be carefully evaluated within this intermediate temperature window, where swelling risk is most severe.

To further quantify this behavior, several empirical correlations for swelling in SS 316 have been developed, most of which describe the dependence on dpa through a polynomial–power law relationship. Among these, a nonlinear regression analysis was performed using Allen's empirical equation [5], and the predicted swelling as a function of dpa is shown in Fig. 1. The polynomial-power model, incorporating a cubic term with five fitting parameters, yielded a root-mean-squared error of 3.265 and an R^2 of 0.979, indicating very good agreement from a general modeling perspective. However, because this formulation employs a single exponential term, it systematically underestimated the nearly constant swelling rate observed after the incubation stage.

To address these shortcomings, a new Incubation–Saturation model was developed. This formulation explicitly incorporates the incubation dpa and represents the ultimate saturation swelling rate using the integral form of a logistic function. A comparison between predicted and measured swelling is shown in Fig. 2, where the saturation effect is more clearly captured than with the polynomial-power model. Model performance was improved, with an RMSE of 1.877 and an R^2 of 0.993.

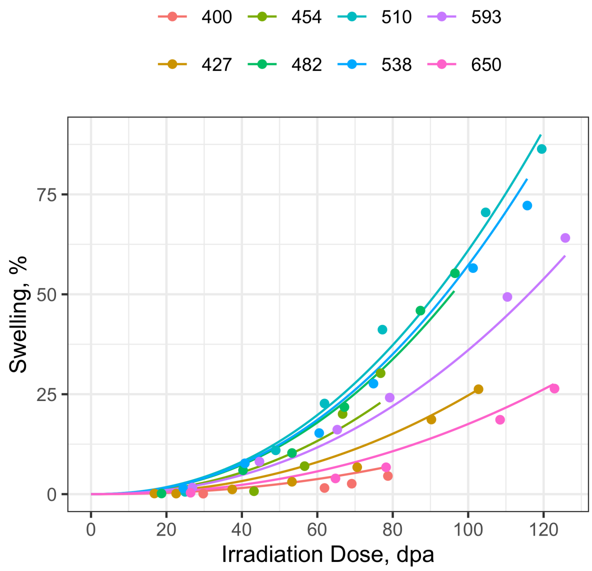

Fig. 1. Comparison of polynomial-power model predictions and measured data for swelling as a function of dpa at different irradiation temperatures.

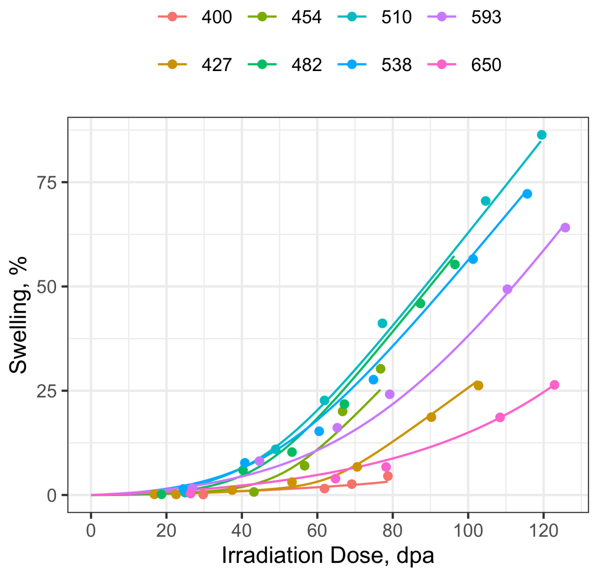

Fig. 2. Comparison of incubation-saturation model predictions and measured data for swelling as a function of dpa at different irradiation temperatures.

Residual analysis (Fig. 3) further illustrates the improvement. Whereas the polynomial–power model exhibited a pronounced wave-like trend in the residuals, the Incubation–Saturation model produced a more stable and random distribution. Nevertheless, the new model, with 11 fitting parameters, carries the risk of overfitting and limited generalization, particularly due to the lack of explicit incorporation of material property effects such as dislocation density, alloy composition, and microstructural evolution. Errors observed in certain temperature ranges emphasize the need for broader datasets, and a mixed-effects framework will be necessary to account for batch-specific variability and to quantify uncertainties. Moreover, the current focus on 20% cold-worked SS316 restricts the model's applicability, highlighting the need to extend future studies to other alloys and irradiation conditions.

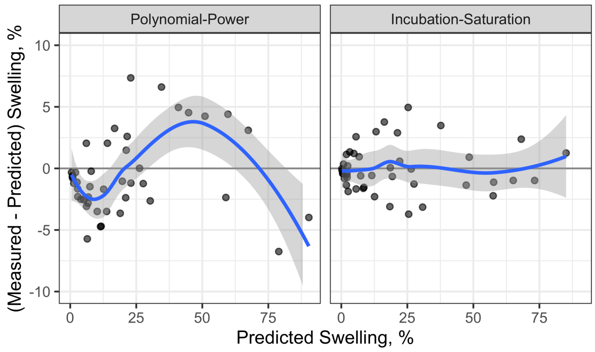

Fig. 3. Residual comparison between the two models. The blue trend lines were obtained using a non-parametric smoothing method.

4. Conclusions

A new swelling correlation was proposed that captures both incubation and saturation behavior, achieving higher accuracy than existing empirical models. The approach demonstrates strong potential for assessing material durability and supporting optimized MSR design, while future work will refine the model through integration of material properties and expanded datasets.

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