Modelling Austenitic Stainless Steels for Fusion Reactors

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Abstract

The irradiation hardening of austenitic stainless steel in fusion reactors has been studied using neural network modeling. The elongation and yield strength have been expressed as functions of different variables such as chemical composition, irradiation condition and other reasonable parameters based on the available database. Problems that occurred in the modeling are discussed and improved models have been built up. The predictive accuracy of the models has been quantified. From these final models, it is predicted that the total elongation of austenitic stainless steel decreases dramatically to below 1% in the environment of high neutron damage and helium production. The conclusion is that these steels are not suitable for use in the first wall of fusion reactors. Suggestions for future work are presented.

Keywords: fusion, irradiation, austenitic stainless steel, neural network, elongation, yield stress

Introduction

Fusion

Fusion power offers the potential for almost limitless energy for future generations but it also presents some formidable scientific and engineering challenges. The heat of the fusion reaction is transferred to an external cooling circuit and the neutrons produced are absorbed by the surrounding materials. Due to the high energy of the neutrons, the mechanical properties of these first walls are affected by displacement damage and the production of transmutation helium. This causes problems such as swelling[1], irradiation hardening[2, 3], irradiation creep[4] and activation.

The irradiation hardening is thought to be caused by an increase in dislocation density and the formation of helium bubbles in the material. Two parameters are very significant in determining the degree of hardening: the amount of neutron damage, measured in displacements per atom (dpa), and the quantity of transmutation helium produced in atomic parts per million (appm). The ratio between them plays a significant role in the microstructural behavior of the materials. In proposed fusion reactors, the neutron damage can be as high as 150 dpa, and the helium/dpa ratio is expected to be roughly 20 appm He/dpa[5]. It is also not yet possible to carry out experiments at the neutron energies expected; a suitable reactor for this will not be available for another 15 years. Therefore, the process of fusion-reactor irradiation damage is studied here using neural network modeling.

Neural networks are capable of investigating problems with large numbers of complex and interacting variables[6] where simplification is unacceptable The creep properties of irradiated steel have been studied previously using this method[7] and the resulting trends were consistent with expected behavior. In the present work, the irradiation hardening of austenitic stainless steel was studied to predict the suitability for use in fusion reactors based on data obtained in fission reactors.

Neural Networks

In this project, neural network modeling is used to predict material properties in damage regions where experimental data does not exist.

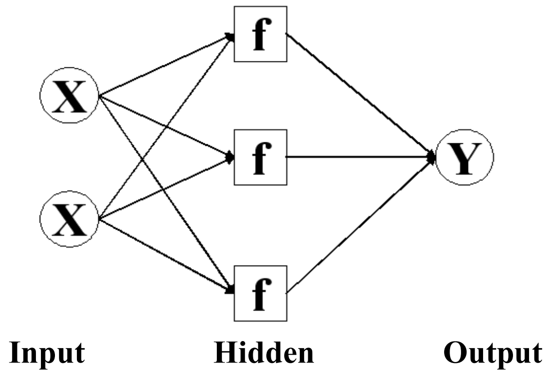


Figure 1. Three-layer structure of neural networks

Figure 1 shows a typical three-layer forward feedback neural network. Information is transferred from neuron to neuron according to the equations below.

$$f_i = \tanh(\sum_i w_{ij}^{(1)} x_j + \theta_i^{(1)})$$

$$y = \sum_i w_i^{(2)} f_i + \theta^{(2)}$$

where w_i and w_{ij} represent the weights and θ and θ_i are biases. Hyperbolic tangent functions are used because, as this function is very flexible, it can fit extremely complex datasets when the weights are properly adjusted. Figure 2 shows an example of an extremely complex contour created using the hyperbolic tangent function.

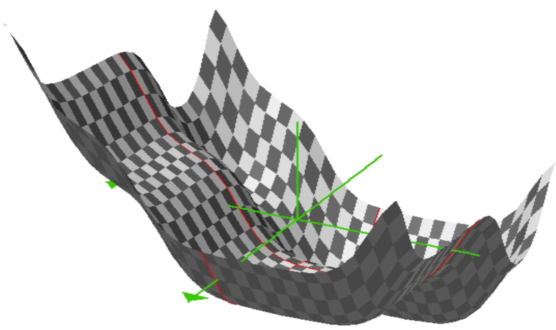
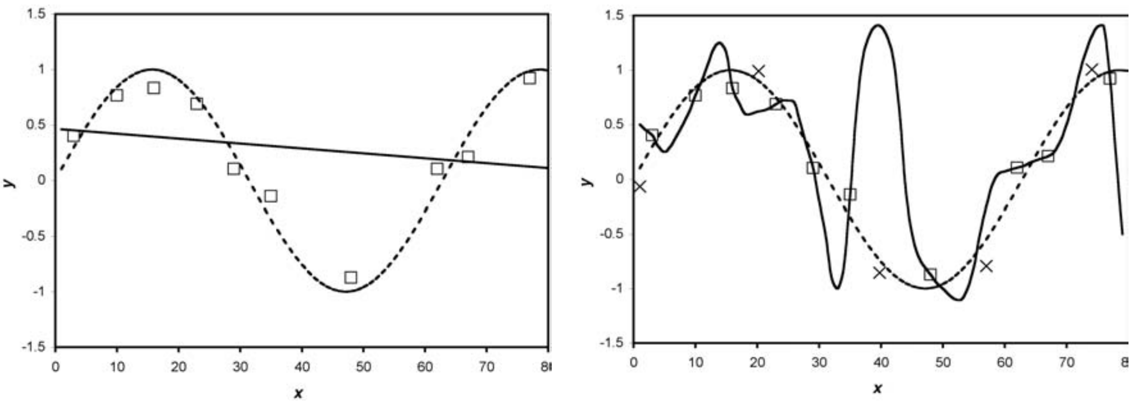


Figure 2. Example of a complex hyperbolic tangent function

Neural network modeling is an extremely powerful tool for analyzing relationships between input and output data. However, its methods and results must always be subjected to "reality checks" to avoid unphysical results. Figure 3 below provides examples of the common problems of "underfitting" and "overfitting" of data. In 3(a), a dataset has been modeled linearly to show the pitfalls of fitting a function that is too simple and missing the general trends in the data. Figure 3(b) shows another problem especially relevant to the hyperbolic tangent. Here, with such a flexible function, it can be made overly complex so that it passes exactly through every data point (square boxes). This will model experimental scatter in the data as though it is meaningful and will again miss the actual trends present in the data and thus prevent accurate extrapolation (crosses).



---- actual trend in data **—— modeling approximation**

Figure 3. Illustrating (a) underfitting and (b) overfitting

One feature of the neural network approach is that it can assemble a committee of submodels. In figure 4, an example plot is included to show that more than one submodel can fit a given set of existing data. Then, in regions where data is sparse or noisy, the various submodels may behave differently. This allows a quantification of the uncertainty of modeling in these regions.

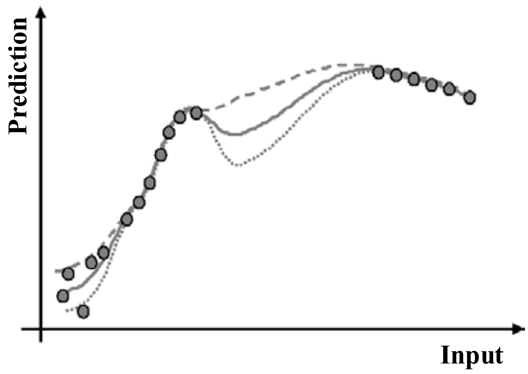


Figure 4. Example of Submodels in a Committee

Procedure

In general, in the neural network approach, models are created, trained and validated. Then they are assessed for possible improvements to input or output parameters to make them more efficient, more accurate or more physically reasonable. Once acceptable models have been produced, these are used to extrapolate from the known data - to carry out "experiments" - to ascertain the properties of the material under conditions which are not available experimentally.

Results

Creating Initial Models

In this project, models were created for total elongation, uniform elongation and yield stress. The first set of models included all information available about the experimental testing. The input parameters are shown on the x-axis of the graph in figure 5 and the output for that model in particular is total elongation. Each model assesses the relative impact of each parameter on the output. The y-axis shows the value of this significance.

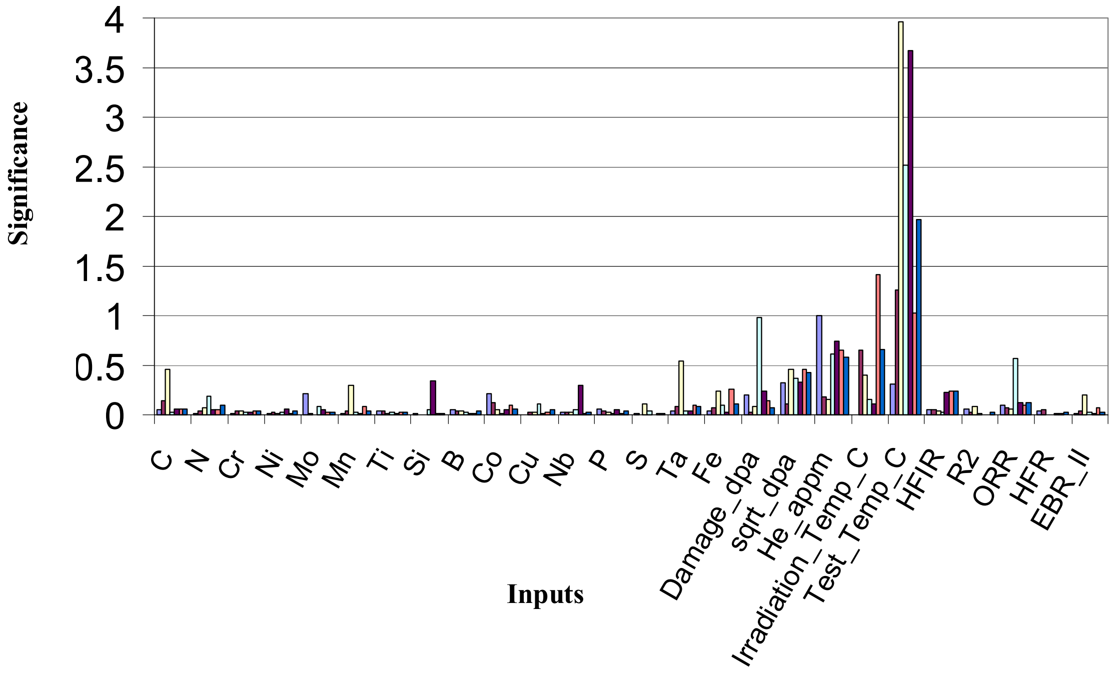


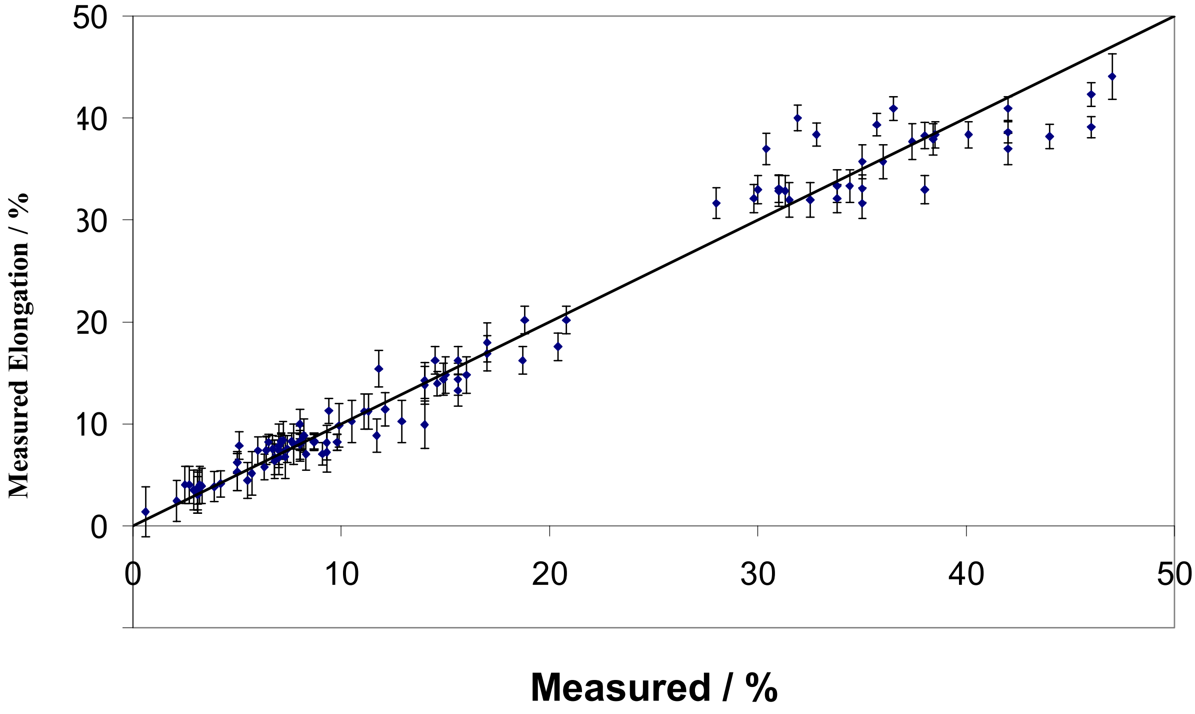
Fig 5. Input parameter significance for a total elongation model

Information for the exact input parameters used in this project are given in table 1 below.

Input variables [units]	**Min.**	**Max.**	**Mean**	**Standard deviation**
Neutron Damage [dpa]	0	44	8.30	8.14
Square root of damage [$dpa^{1/2}$]	0	6.63	2.31	1.72
Helium production [appm]	0	3488	242.79	576.48
Transmutation ratio [He appm/dpa]	0	79.55	14.46	22.58
Irradiation temperature [K]	298	983	511.53	170.35
$Exp(-1/T_{irr})$	0.9966	0.999	0.9978	0.0008
Test temperature [K]	473	973	612.55	121.99
$Exp(-1/T_{test})$	0.9979	0.999	0.9983	0.0003

Table 1. Statistics for the values of the input parameters [Note that information regarding composition and reactor data is not included, as explained later.]

As mentioned, once a model has been created, its validity must be tested. A very useful "quick look" test is to have the model make predictions on the training dataset. The predicted values should reflect trends that existed in the measured data and therefore the model should predict similar values. The model will generally not predict the exact outputs that were measured - this would be an indication of overfitting. The chart of predicted and measured data (shown for total elongation in figure 6) illustrates the comparison between the model's output and the actual values. For the total elongation case, the computed and measured values match closely, with a correlation coefficient of 0.9868.



Measured Elongation / %

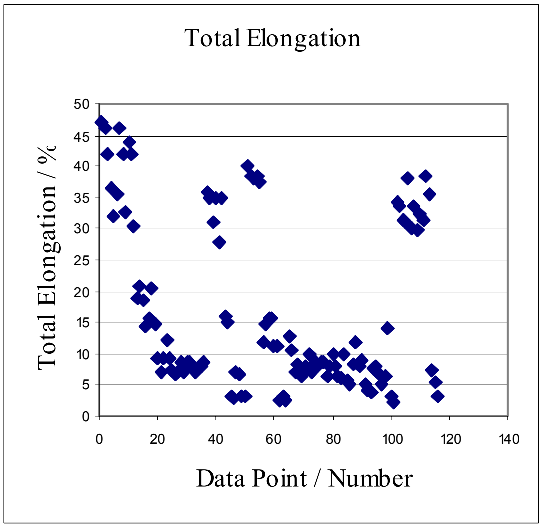
Figure 6. Validation of the total elongation model

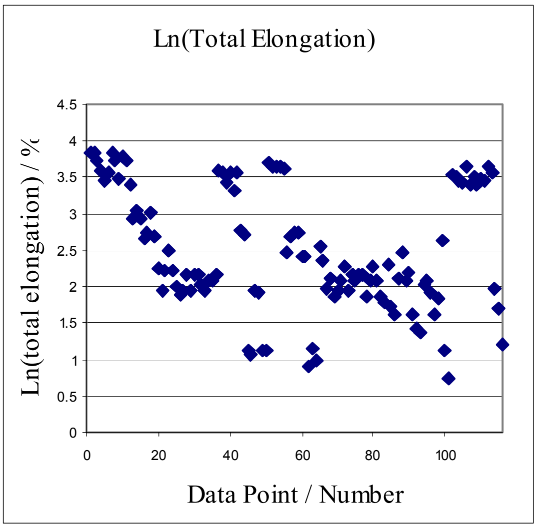
The error bars at each data point represent the uncertainty of modeling for a given value. The probability of a particular model giving the training data (the data is assumed to be noisy) is calculated using a Bayesian approach, and these probabilities are summed across all models to give the total uncertainty. The uncertainty of modeling for this total elongation model in particular was reasonable, on the order of 10%.

Improving the Models

Once initial models were created, they had to be analyzed to identify where improvements could be made. The first significant issue to be addressed was the ability of the models to predict negative elongations and yield strengths. Since a neural network outputs numbers without "knowing" the details of the parameter being modeled, it can and will give unphysical outputs unless prevented from doing so. Another significant issue arises from clustering of data in input space. This may cause the model to interpolate linearly between two clusters thereby ignoring real underlying trends in the data. This highlights the importance of how data is presented to the neural network.

For example, in figure 6(a), the data for total elongation shows clustering as there is a large amount of data below 20% and above 30%, but almost no points in between. This issue can be addressed by using the natural log of elongation as the target for the model rather than the elongation itself. Figure 6(b) contains the same data, but shows that it can be presented to the model with continuously varying values over the output space by using the logarithm. The exponent of the output from the model is then taken, returning the output data to meaningful values of elongation. Incidentally, this also solves the problem of negative model output, as the exponent of any number is always greater than zero.





<u>Figure 7. Illustration of (a) data clustering and (b) improvements made with natural log</u>

Further improvements were made to the model by refining the input parameters. From the chart of significances for total elongation (figure 7), it is clear that input data regarding both composition and reactor used have far less importance than any of the other parameters. These inputs had coefficients of 0.1 or less, whereas in comparison the significance of the other inputs varied from 0.25 to 4.0. This is to be expected, as while in general composition has a significant effect on the mechanical properties, in this case the compositions varied so little that the model effectively treated their values as constants. Therefore in subsequent models, the composition and reactor inputs were removed to make the model more efficient without any significant loss in accuracy.

Further improvements were made by adding mathematical expressions containing input parameters that may have relevance to the output. This helps the neural network to detect non-linear dependencies on input parameters or on relationships between two or more such inputs.

An Arrhenius-type relationship for temperature was added as a parameter for both irradiation temperature and test temperature to detect any energy-activated processes, as are known to occur in creep. Such relationships can be added safely, as the neural network is capable of ignoring extraneous parameters.

The helium to damage ratio (He/dpa) was also added to the input database, as this is frequently quoted in the literature as having an effect on mechanical properties and can also change according to the energy spectrum of neutrons in a reactor and the steel involved[8]. This has the added advantage of incorporating indirectly in this input parameter the neutron fluence; data which was not provided for the experiments.

Another parameter was added to account for the hardening due to the difficulty of dislocation motion induced by the helium bubbles. This parameter is 1/L, the inverse of the average spacing between the bubbles. The computation of this parameter is complex and some of the relevant equations are contained in Appendix I. And finally, $\sqrt{dpa}$ was added as it is related to the nucleation rate of the helium bubbles[9].

It must be noted, however, that while adding parameters such as the square root of damage can significantly improve the accuracy of a model, it should be added in addition to dpa. Mathematical expressions containing inputs may be added in conjunction with the raw input, but must not replace it. Otherwise the model may be biased and misinterpret certain trends.

Final Models

After various iterations of improvements, final models for uniform and total elongation as well as yield strength were created. The yield stress model had excellent agreement between the measured and predicted values, with a correlation factor of 0.9869 and an average error of just 3.6%. However, although this model performed extremely well in the region where data existed, problems arose upon extrapolation of the yield stress values to damage regimes similar to that sustained by an actual fusion reactor first wall.

As illustrated in figure 8 below, the yield strength of the steel is predicted to rise sharply with initial irradiation damage, but to decrease to well below the unirradiated value at higher doses. This does not make physical sense. The actual yield stress increases with dpa as is suggested by the experimental fission data and explained in the literature [10]. While there can be softening effects due to irradiation damage in certain cases, this has only been observed at temperatures greater than ~773K.[11]

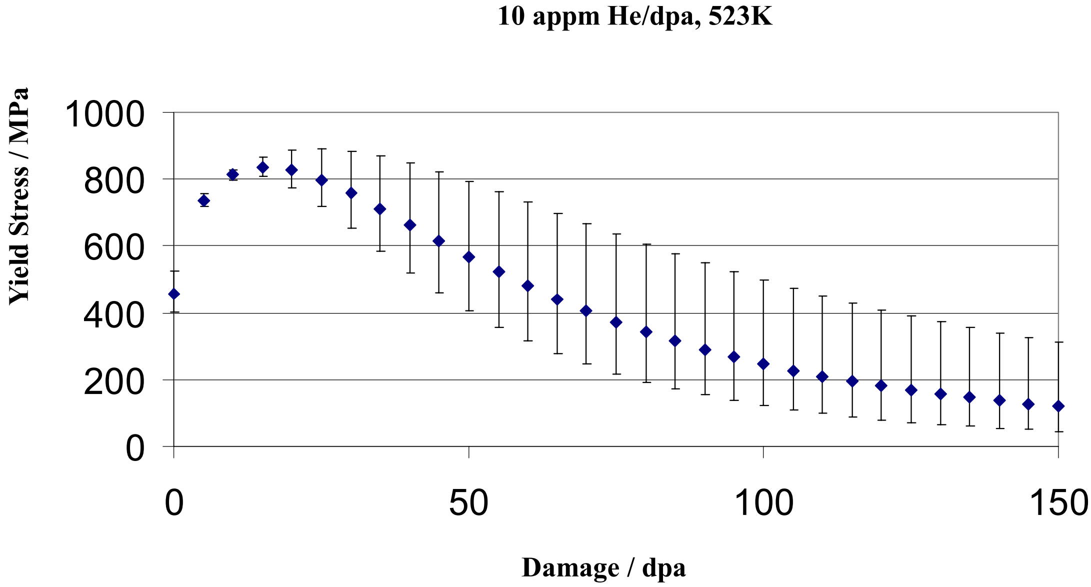


Figure 8. Yield Strength Predictions with the 1/L input parameter

To investigate where the model was going wrong the input parameters were checked. Upon further examination it became apparent that at higher damage rates, the calculated values of L were becoming unrealistic. The size of the He bubbles was calculated to be on the order of the average spacing between them. It was concluded that the approximations implicit in the calculations were not valid in the relatively poorly-understood regions of extremely high irradiation damage. Therefore 1/L was removed as an input for all models. In the absence of the 1/L input parameter, the yield strength predictions track much more closely with theory.

After removing the 1/L parameter from these final models for total elongation and yield stress, the results were very reasonable and accurate. However the model for uniform elongation had problems throughout the project. This model was initially created with exactly the same database of inputs as the total elongation (which behaved) and the outputs were taken from measured experimental data. However the various members of the committee were not in good agreement and the model had serious flaws. In validation of the model, the predicted and measured values were in good agreement, having a correlation of 0.9771. But, despite this agreement, there was a large degree of uncertainty of modeling - on the order of 35% (figure 9). Further, the predictions for the uniform elongation in a high damage region are meaningless as is shown below in figure 10. The experimental data clearly indicates that the uniform elongation is expected to decrease with increasing damage and, under no circumstances, should it blow up to far greater than 100%.[11]

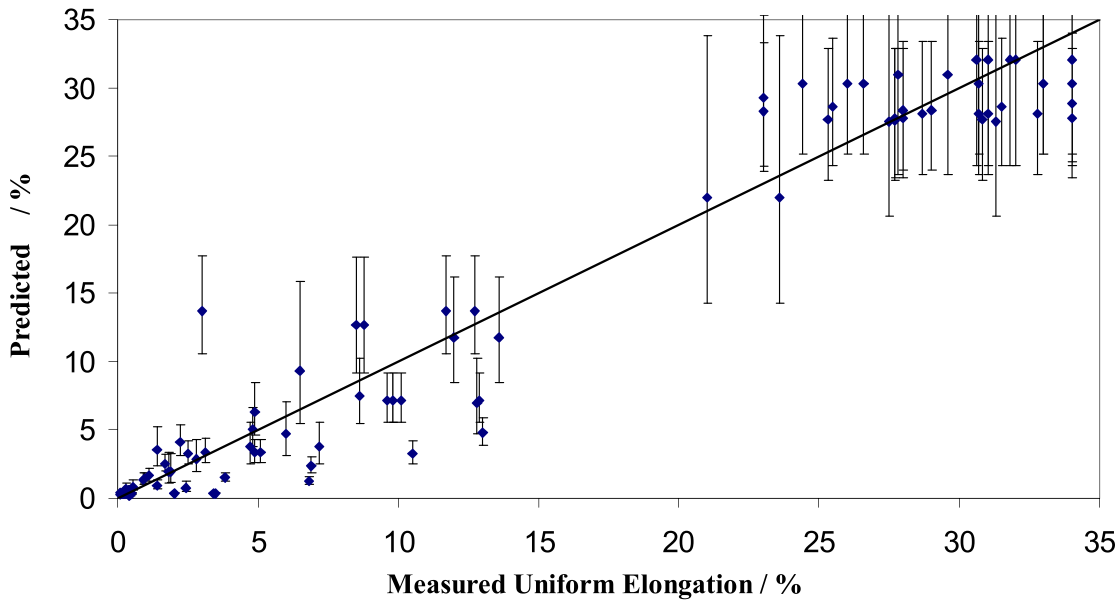


Figure 9. Uniform elongation model validation

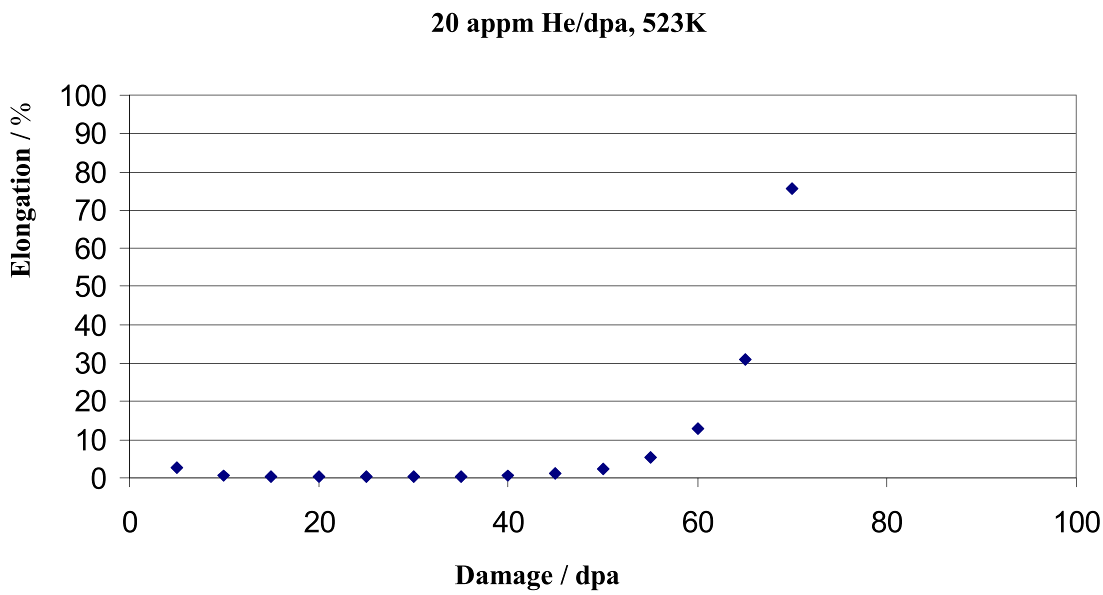


Figure 10. Predictions for the uniform elongation model

Discussion

Model Predictions and Analysis

The total elongation model was far better-behaved than the uniform model. When testing this model, there was good agreement between the predictions and the measured values, with a correlation coefficient of 0.9678. And, unlike the uniform elongation model, this model had a more reasonable error of roughly 10%. This model had been validated and was able to make meaningful predictions about the suitability of austenitic stainless steel for use in a fusion reactor first wall. These predictions of total elongation are shown in figure 11. The significant result is that this model definitively predicts that these steels would be too brittle to be used for this purpose. The ductility drops to less than 1% for 100 dpa and less than 0.5% for 150 dpa. This simply will not meet the design criteria for the materials needed.

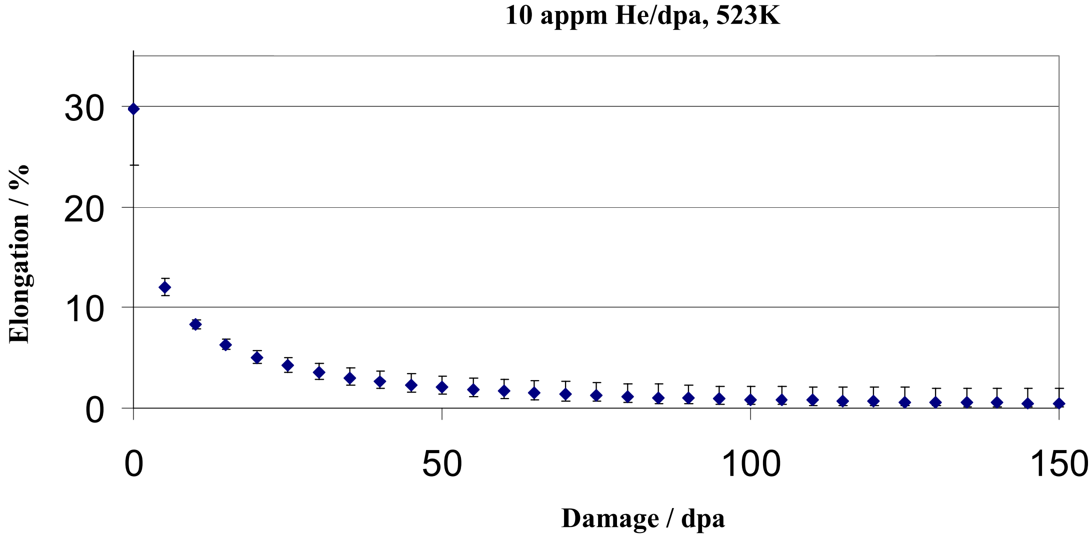


Figure 11. Predictions for total elongation with increasing irradiation damage

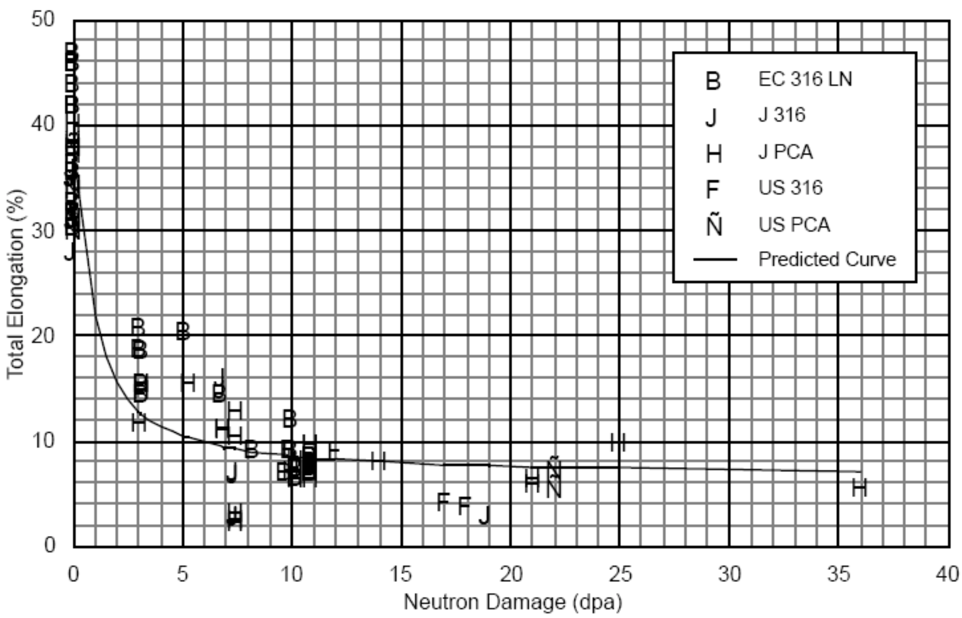


Figure 12. Measured Values of Total Elongation in the Fission Region

This is an important and physically reasonable result. Nevertheless all predictions made by neural networks must be compared with established trends to verify that they are reasonable. This sharp decrease in elongation with damage is confirmed by the experimental data from the fission regime, as shown in figure 12.

This sharp decrease in elongation is consistent with an increase in yield strength with damage. This was successfully predicted by the yield strength model as is shown below in figure 13. This model was also very reliable, having a correlation coefficient between measured and predicted values of 0.9871, with an average error of just 3.5%.

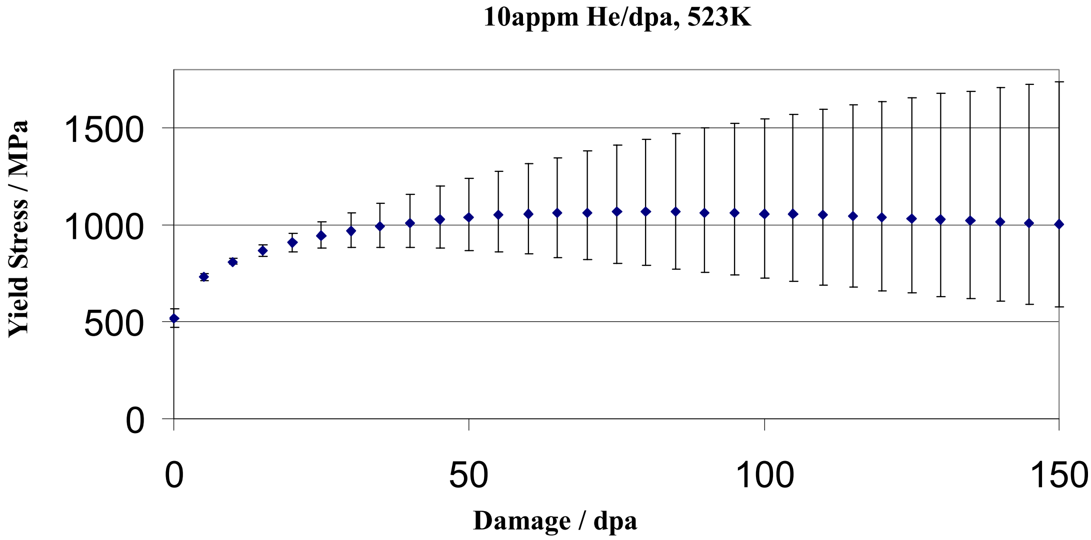


Figure 13. Predictions from the yield strength model

Suggestions for Future Work

One obvious difficulty of this project was encountered in creating an accurate model for uniform elongation. Of the five models created for this output, all had high levels of uncertainty and made predictions that ran counter even to the trends in the fission regime where data exists. With more time, this output would have been more thoroughly investigated and the root cause of the problem might be found.

While the results presented in this report seem reasonable, predictions from modeling should ideally be tested experimentally before they are completely trusted. One suggestion for future work is to do this, but unfortunately an experimental reactor capable of creating fusion conditions will not be ready for some fifteen years. This means that relevant experimental data cannot be obtained at present, neither for the purpose of validating the predictions presented in the current report, nor for providing data for further models.

One suggestion for general improvement of irradiation experiments became apparent as much of the reported information tends to be incomplete with many potentially important parameters left out. Since the entire topic of irradiation at high levels of damage is still not well-understood, every effort should be made to carefully control and report on all possible data. For instance, the neutron energy spectrum to which the material has been exposed is not frequently given even though it is generally recognized[10] that this is factor has a considerable effect upon the characteristics of the material. In particular, the models presented here would be significantly improved if information regarding the microstructure and the heat treatment received for each steel were able to be included as inputs. Elongation in general depends on dislocation motion and a parameter such as average grain size can be extremely important. Nevertheless, given the lack of this type of data, the models were still able to make meaningful predictions. This is an illustration of the power of neural networks.

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Appendix I

As previously described, the helium bubbles can be considered as very small and finely dispersed impenetrable barriers to dislocation glide.

The bubble number density equation used was:

$$N_c = (5.36*10^{12}) \exp\left(\frac{1.15eV}{k_B T}\right)$$

If all the He is uniformly distributed between these bubbles at these trapping sites then at the end of the irradiation period each bubble will contain:

$$N_G = \frac{N_{HE}}{N_C} \text{ atoms of He}$$

It can be assumed that the bubbles are at equilibrium pressure (use the Van Der Waals equation of state to balance the He gas pressure against the inward pressure of the interior surface (surface energy $\gamma = 2\ Jm^{-2}$).

$$P_G = \frac{n_G k_b T}{\frac{4}{3}\pi r^3 - b_v n_G} = \frac{2\gamma}{r}$$

The exact solution to this cubic equation for the equilibrium bubble radius r_{eq} is given by

$$r_{eq} = \frac{2\pi\gamma k_b T n_G + \left[24 b_v \pi^2 \gamma^3 n_G + \sqrt{576 b_v^2 \pi^4 \gamma^6 n_G^2 - (2\pi\gamma k_b T n_G)^3}\right]^{2/3}}{2\pi\gamma\left[24 b_v \pi^2 \gamma^3 n_G + \sqrt{576 b_v^2 \pi^4 \gamma^6 n_G^2 - (2\pi\gamma k_b T n_G)^3}\right]^{1/3}};$$

Where,

- b_v, Van Der Waals Packing Volume
- γ, Surface Energy = $2Jm^{-2}$
- k_b, Boltzmann's Constant
- T, absolute temperature
- N_G, Number of helium atoms per bubble

It can be assumed that there are two dominant hardening effects: a change in the yield stress caused by an increase in dislocation density and a change in the yield stress caused by the formation of Helium bubbles.

i.e. $\Delta\sigma_y^2 = \Delta\sigma^2_{y,\ \text{dislocations}} + \Delta\sigma^2_{y,\ \text{bubbles}}$

The general form for hardening caused by a distribution of obstacles is proportional to 1/L where $L = (N_c d)^{1/2}$

Thereby, disregarding the increase in yield stress due to the increase in dislocation density:

$$\Delta\sigma_{y,\ \text{obstacles}} \propto \frac{1}{(N_C d)^{-\frac{1}{2}}} = 1/L$$