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Designing Optimised Experiments for the International Fusion Materials Irradiation Facility

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Abstract

The development of fusion power requires a facility for assessing the behaviour of materials subjected to damage from 14 MeV neutrons with displacement damage levels of up to 150 atomic displacements per atom. The proposed International Fusion Materials Irradiation Facility (IFMIF) will enable experiments to be conducted that closely fit these requirements.

When designing experiments it is at first sight natural to suggest a uniformly sampled test matrix over the domain of interest. However, as the irradiation volume in IFMIF will be limited, it is appropriate to consider how the set of experiments may be optimised.

In the present work we suggest a set of experiments designed using predictive Bayesian neural network models created using published data for irradiated reduced-activation martensitic steels. It has been possible to identify gaps in knowledge on the basis of model-perceived uncertainties, and to access trends in order to determine more optimal sampling of experiments.

Keyword codes

L0400, M0200

1. Introduction

There are various key unresolved issues in the modelling of irradiation effects on materials for use in future fusion power plants [1]. One of these is the extrapolation of models - based on observations of materials irradiated in current lower-energy facilities and fission reactors - to the high-energy, high-dose fusion-relevant regime. The proposed International Fusion Materials Irradiation Facility (IFMIF), when built, will provide suitable experimental facilities for testing the predictions of mechanistic models on candidate power plant materials by simulating a fusion irradiation spectrum [2]. However, the available experimental volume in the high-flux region in IFMIF is ~ 0.5 litres, and the highest-damage (≥ 150 atomic displacements per atom (dpa)) experiments will last 5 years or more, meaning that experiments must be carefully chosen to make the best use of this space.

Ideally, the behaviour of radiation-damaged materials could be predicted mechanistically. However, these effects are complex and involve many variables whose roles are not fully understood, and ignoring the effect of any of these variables could lead to an unacceptable oversimplification of the problem and hence inaccurate predictions [3]. Examples of material properties that cannot be predicted from first principles are yield stress and fracture toughness - models exist which can give qualitative predictions of changes in these properties, but cannot provide the quantitative predictions vital to successful engineering.

We have modelled tensile and Charpy properties for irradiated low activation martensitic (LAM) steels using an artificial neutral network (ANN) approach [4, 5]. The modelling method has been described previously; it suffices to say here that it is based on a Bayesian inference method which gives as outputs not only a numerical prediction, but also the important *modelling uncertainty* in that prediction which includes experimental noise, the ability of the network to "fit" the data, and how far outside the limits of the input database predictions are being made.

Interest is focused on two of the most promising of the LAM steels, Eurofer (9-Cr) and F82H (8-Cr).

2. Model predictions at low dose

It is clear from model predictions (Fig 1) that the most rapid period of variation in the properties of an irradiated LAM steel is during an initial low-dose period, less than 5 dpa. The rate of change of these properties with dose also depends strongly on irradiation temperature. In addition, although modeling uncertainties are generally small in the low dose regime, it should be borne in mind that these predictions are based on data gathered from non-fusion spectrum sources.

Studying the relevance accorded by the ANN to various inputs, it is also clear that the property variations are more strongly correlated with functions such as the square root of dose, rather than with the dose itself (Fig 2) [4].

In combination, these effects suggest that the sampling distribution of doses chosen for the proposed experimental matrix should be weighted towards lower dose experiments with a smaller number of high-dose specimens. This will have the two-fold benefit of providing more data at an early stage - allowing the validation of models - and maximising the effective spread of the data.

In addition, the temperature region from 250 - 550ºC is the region where radiation effects on the yield stress and Charpy toughness are most marked, and one that encompasses the proposed blanket temperatures of fusion plant - although a comment should be made on the possible occurrence of temper embrittlement (caused by the segregation of phosphorous to grain boundaries at temperatures around 600ºC) [6]. Behaviour typical of this sort of high-temperature embrittlement has been detected in the ANN models (Fig 3).

3. Model predictions for the fusion regime

It can be seen (Figs 1 and 4) that the ANN model predictions become increasingly uncertain at high dose (particularly above 50 dpa). This is accompanied by a range of predicted behaviours, including saturation and recovery, particularly at elevated (> 500ºC) irradiation temperatures. Both effects are physically justifiable (in terms of the formation and subsequent annealing of extended microstructural defects such as dislocation loops *etc.*), but the present data do not allow the two effects to be separated and so allow us to predict which will dominate under fusion-spectrum irradiation. It will therefore be useful to maintain a number of higher-dose experimental points to "pin" such ANN models and hence lower uncertainties.

We are currently working to incorporate what data there is available on helium effects into the models, and hence to quantify this important additional factor.

4. Comment on model inputs

Neural network training is, effectively, a method of multi-dimensional non-linear regression. In a complex problem, such as the modelling of Charpy toughness of an irradiated material, errors and uncertainties can be introduced by lack of information. The size of the training database is a balance between available, incomplete, data (which are perhaps missing complete compositional information, for example) and a shortage of completely described experimental points. Some of these issues are described in a previous paper [5], but we repeat it here - it is vital that published results include or lead to full descriptions of materials and experimental set-up. It is also true that in some cases, experimental results cannot be "normalised" for comparison with others - the value of the Charpy ductile-to-brittle transition temperature (DBTT) for a particular material is in part a function of specimen size and geometry, for example, rather than a true material property. It is therefore important that a standard geometry is consistently applied, so that results from different experiments can be constructively compared.

5. Summary and conclusions

Neural network models for the effects of irradiation on yield stress and Charpy DBTT of LAM steels have been constructed. Examination of the trends and associated outputs from these models leads us to the following conclusions:

- Having demonstrated that higher temperature (T > 550ºC) effects such as temper embrittlement are present in the data, the experimental regime should extend to at least 600ºC in order to cover these effects.
- Target experimental doses should be chosen to reflect suspected underlying physics, such as the function sqrt(dpa). In this case, picking eight target experimental doses (for each temperature, as per [7]) between 5 and 150 dpa gives 5, 13, 26, 43, 63, 88, 117, and 150 dpa.
- The models show the sensitivity of DBTT and YS to all the inputs, highlighting the need to report experimental data as fully as possible.

Future work will include using these models to explore the significance of other physically significant inputs (such as the commonly used - for heat treatments such as tempering - *kinetic time*: $t\exp(-Q/kT)$. For irradiation damage the substitute *dose* × $\exp(-Q/kT)$ is suggested, where Q is a suitable activation energy for microstructural evolution) to further refine the experimental matrix with respect to dose/temperature interaction. We also intend to use the models to suggest a composition and heat-treatment for an optimised LAM steel for consideration as a power plant material, and hence for IFMIF experimentation.

Acknowledgments

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Figure captions:

Fig 1: Model predictions for variation of DDBTT and YS as a function of dose (see references [4] and [5] for full explanations of these figures).

Fig 2: Neural network perceived significances for selected inputs to Charpy DDBTT (left) and YS (right) models. These significances are akin to partial correlation coefficients [4, 5].

Fig 3: Model predictions for an F82H-based alloy with varying phosphorous content, irradiated to 2.5 dpa at different temperatures. The markedly different behaviour at 600ºC is characteristic of temper embrittlement.

Fig 4: Hardening prediction (and associated modelling uncertainty) for Eurofer as a function of temperature ($T_i = T_{test}$) and dose [5].

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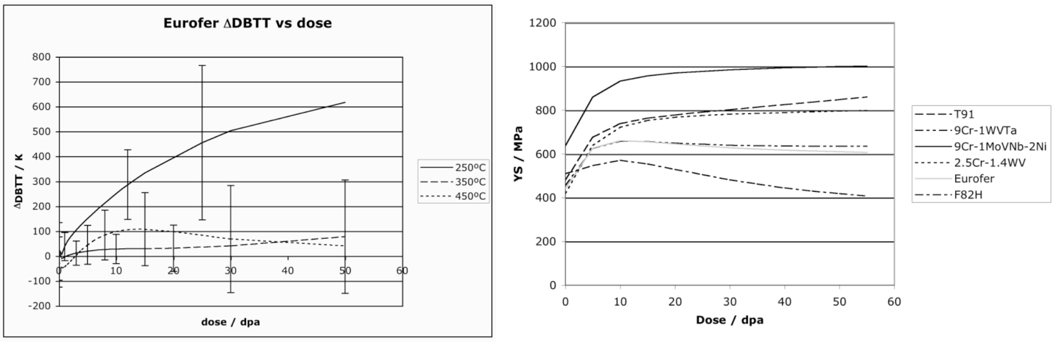

Fig 1

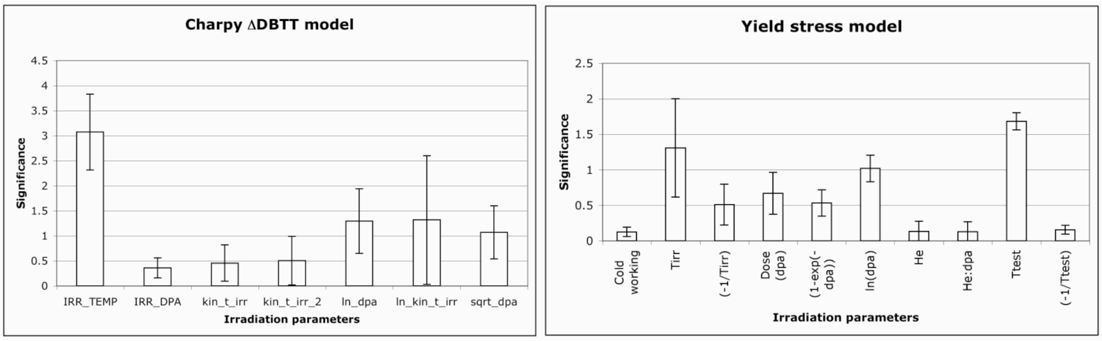

Fig 2

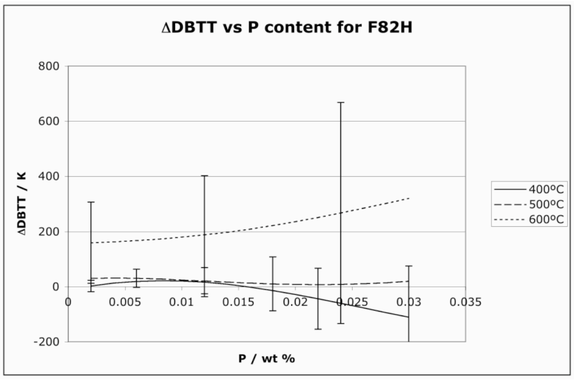

Fig 3

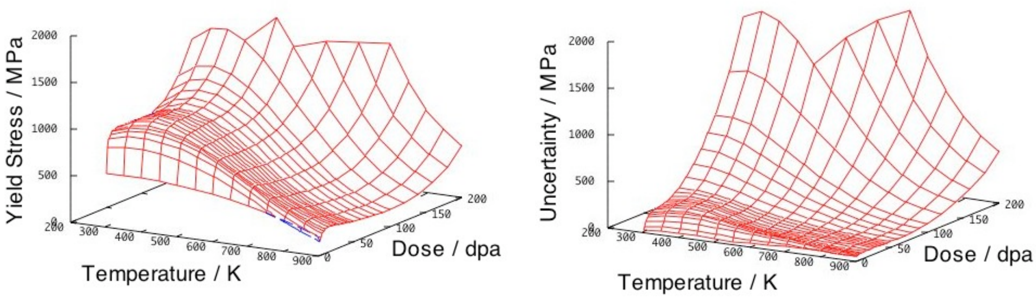
Yield Stress / MPa
2000
1500
1000
500
0
200
300
400
500
600
700
800
900
Temperature / K
0
50
100
150
200
Dose / dpa
Uncertainty / MPa
2000
1500
1000
500
0
200
300
400
500
600
700
800
900
Temperature / K
0
50
100
150
200
Dose / dpa

Fig 4