Extrapolating sparse data: predicting materials properties for a fusion power plant

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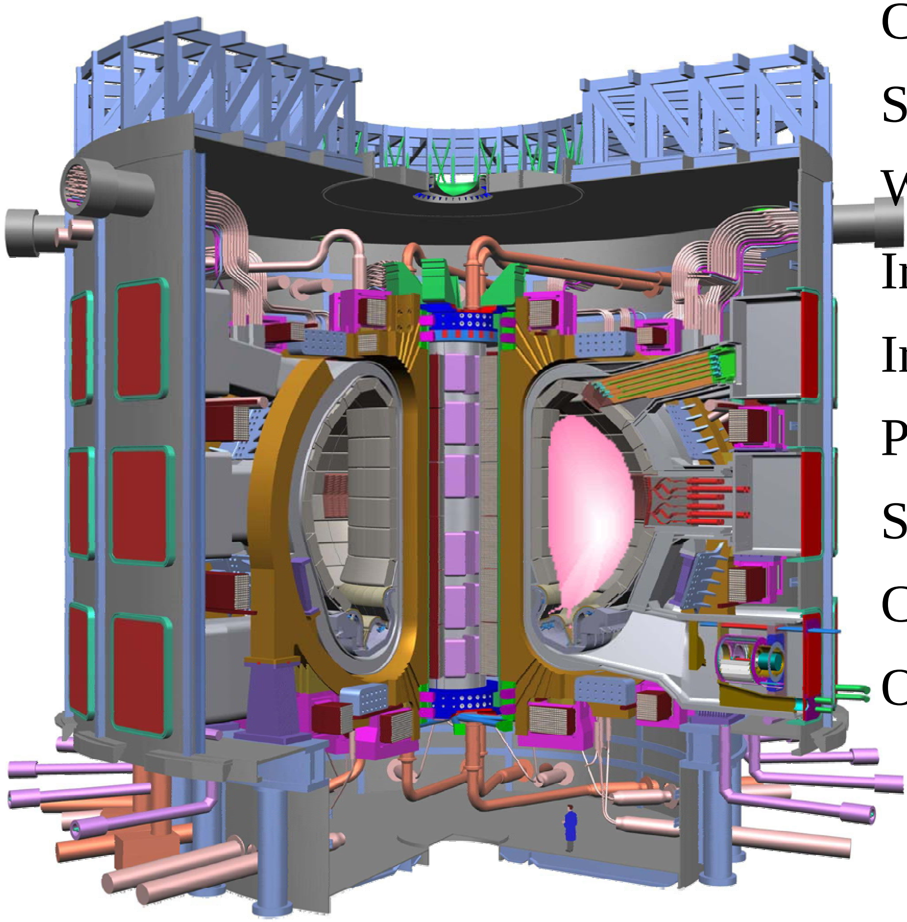
Outline

"Fusion will be ready when society needs it"
Lev Artsimovich (~1972)

- The materials conditions likely within a fusion power plant
- Metallurgical knowledge: the yield stress and Charpy toughness in low activation ferritic martensitic irradiated steels
- Neural networks in an extrapolation mode: dimensionality reduction: complexity optimisation
- Predicting the most suitable alloys from existing data: Benefit functions for yield stress, Charpy and activation

ITER



Major radius 6.2 m: Minor radius 2.0m

Construction costs £5 Billion in 10 years

Stainless Steel 316L-IG components

Wall load 0.5 MWm^{-2}

Irradiation level: about 4 dpa in lifetime

Irradiation temperature about 300 ^{o}C

Pulse length: about 1000 secs

Site in France (Cadarache) chosen 2005

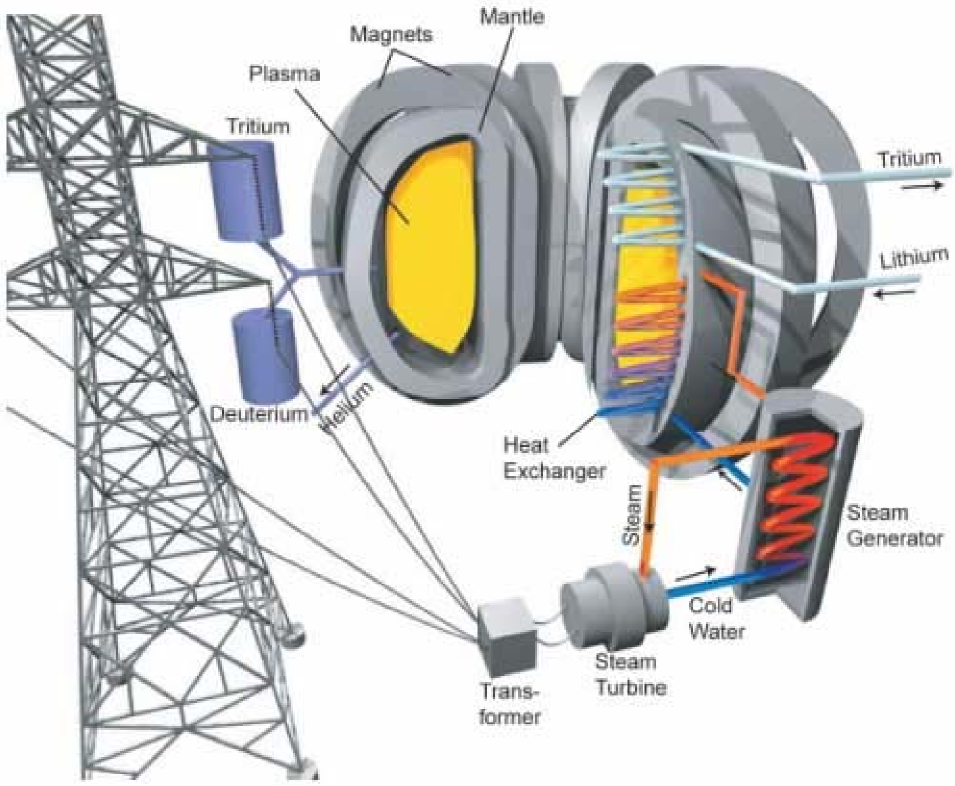
Construction started 2008

Operations due to commence 2018

Aim – to demonstrate integrated physics and engineering on the scale of a power station

Funded by Europe, Japan, Russia, US, China, South Korea and India

Power Plant Conceptual Study (B)



Major radius = 8.6m Minor 1.9m

Continuous operation

Fusion power 3.6GW

Net electrical power = 1.3 GW

Power cycle efficiency = 36%

Wall load 2.0 MWm-2

Irradiation over component lifetime:
about 40 dpa for divertor:
around 100 dpa for blanket

Irradiation temperature about 400C

"A Conceptual Study of Commercial Fusion Power Plants" EFDA-RP-RE-5.0, (2004)

Predicting the metallurgical properties of highly irradiated steels from measurements at lower irradiation

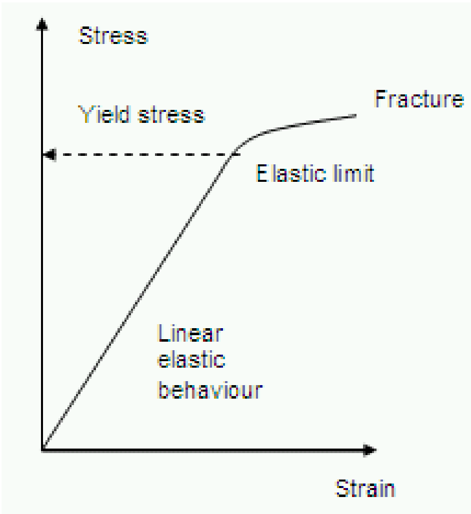
Use existing databases for the properties of irradiated ferritic steels in collaboration with Prof Bhadesia's group at Cambridge

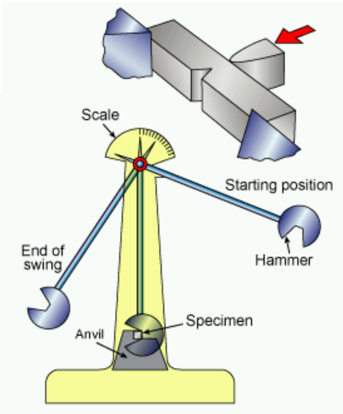
We use neural networks trained at low irradiation levels,
say <40 displacements per atom (dpa),
to predict the properties,
say yield stress and Charpy toughness, at the levels of irradiation (~40 dpa or higher) of the fusion power plant

Colin Windsor, Geoff Cottrell and Richard Kemp, "Prediction of yield stress in highly irradiated ferritic steels" Modelling Simul. Mater. Sci. Eng. 16 (2008) 025005 , stacks.iop.org/MSMSE/16/025005:
"Prediction of the Charpy transition temperature in highly irradiated ferritic steels", Modelling Simul. Mater. Sci. Eng. 16 (2008) 075008. stacks.iop.org/MSMSE/16/075008/

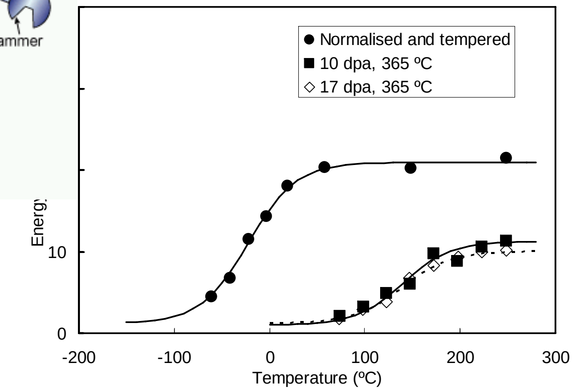
The yield stress and Charpy shift

A stress rig





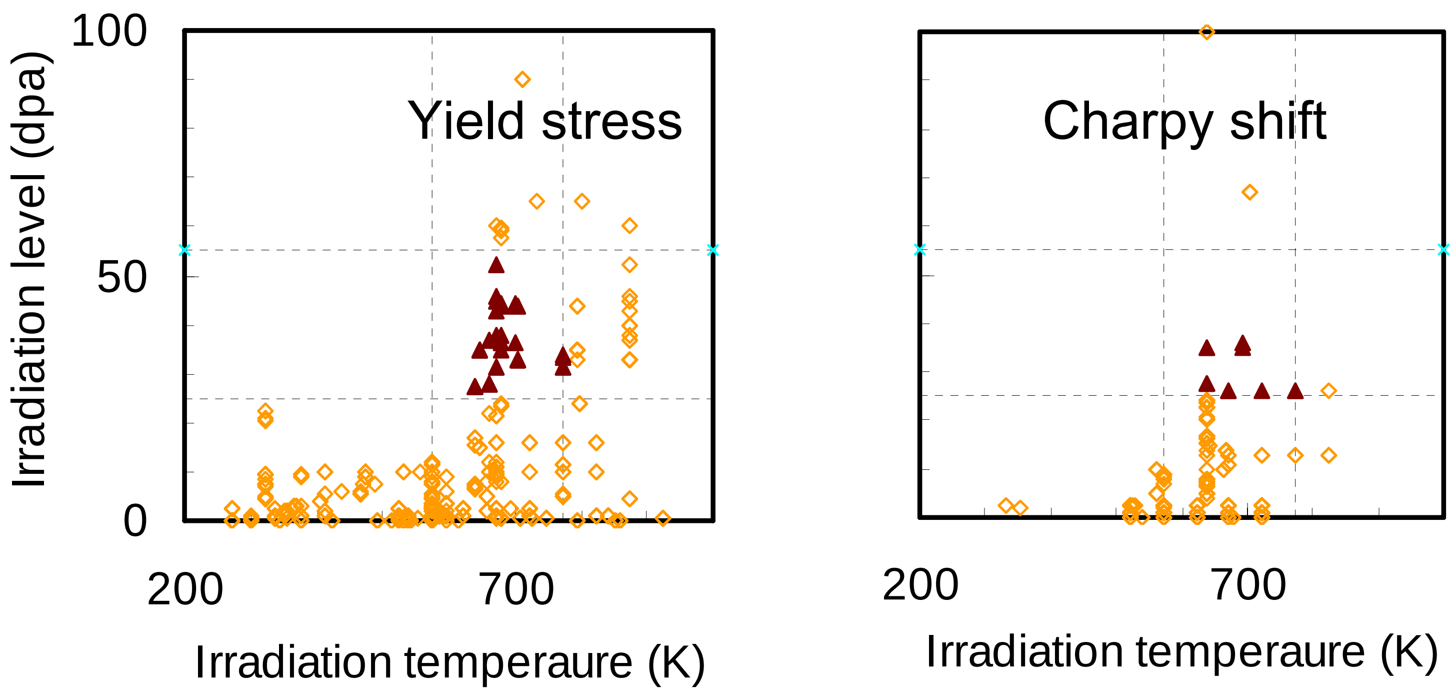
A Charpy
impact tester



The yield stress measures the maximum **strength** of a material while it behaves elastically.

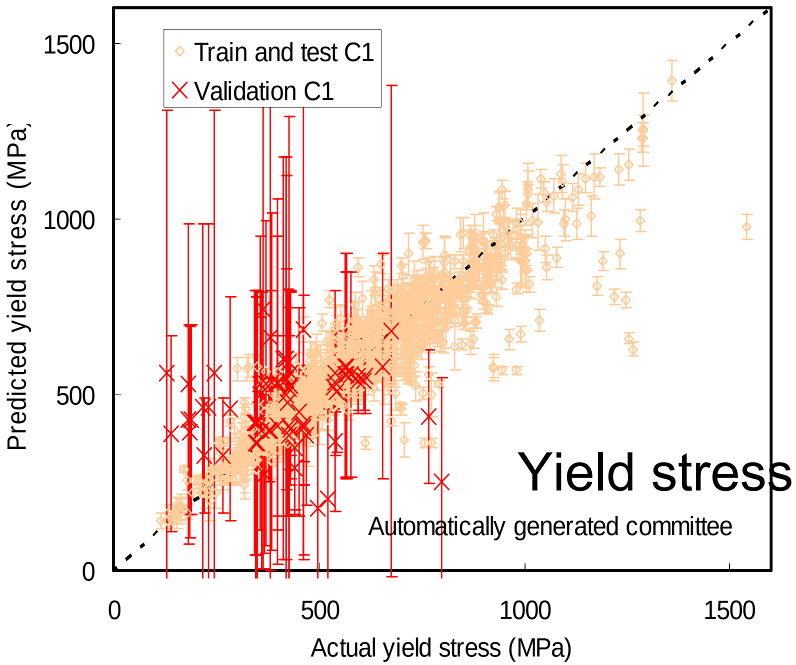
The Charpy shift measures the change of **toughness** of a material under irradiation. Irradiated samples are sub-size.

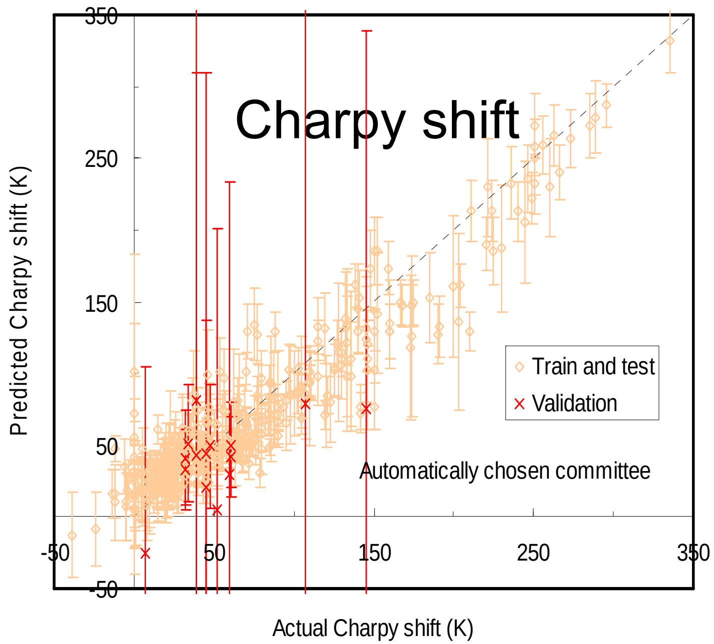
Fusion reactor relevance



The plot shows the limited information at fusion reactor levels, which we define as say from 25-55 dpa and 300-500 K.
For more data we have to wait for ITER (2018) or IFMIF (even later)
For now we can train a network outside this range (open symbols) and Test within the range (closed symbols)

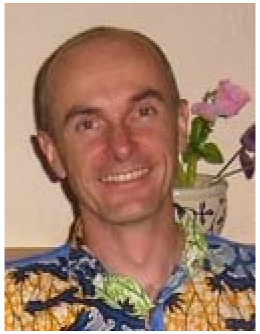
High irradiation results (BIGBACK)





Thomas Bayes
1702-1761

These neural net fits were trained with a 50% selection of data outside the reactor relevant region and tested with the remainder. The committee automatically optimised the fit. The validation data lay within the reactor relevant region. The Cambridge Bayesian code of David MacKay was used.

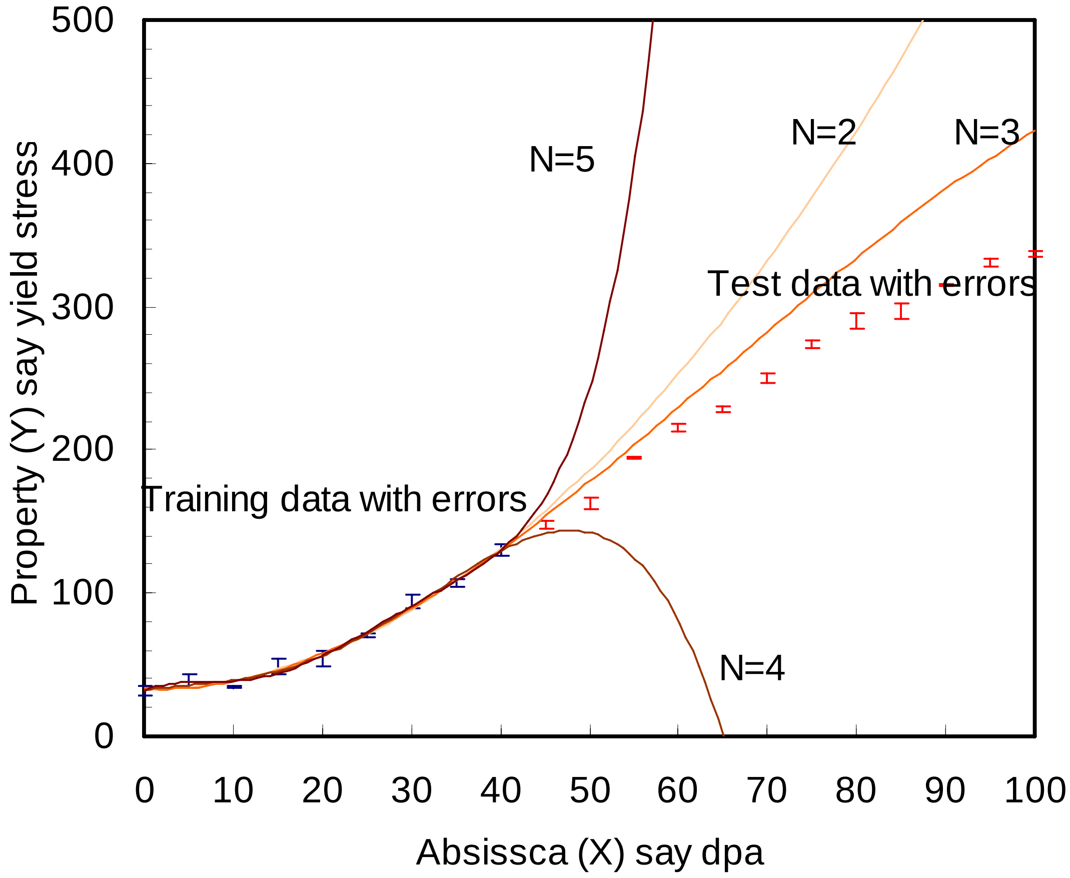


Extrapolation is not easy!

The points are a 3rd order polynomial with imposed random deviations

The blue points below 40 are used for training

The lines are polynomials fitted to the training points with the order shown



Dimensionality optimisation

In difficult "extrapolation" conditions, there is a need to use fitting processes which appropriately reduce the number of adjustable variables.

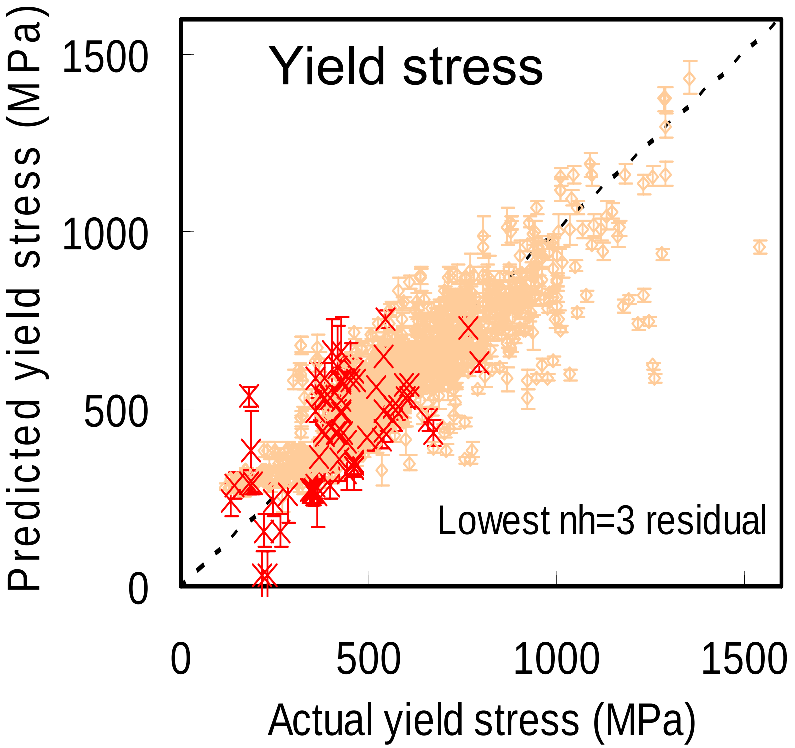
Several methods may be used:

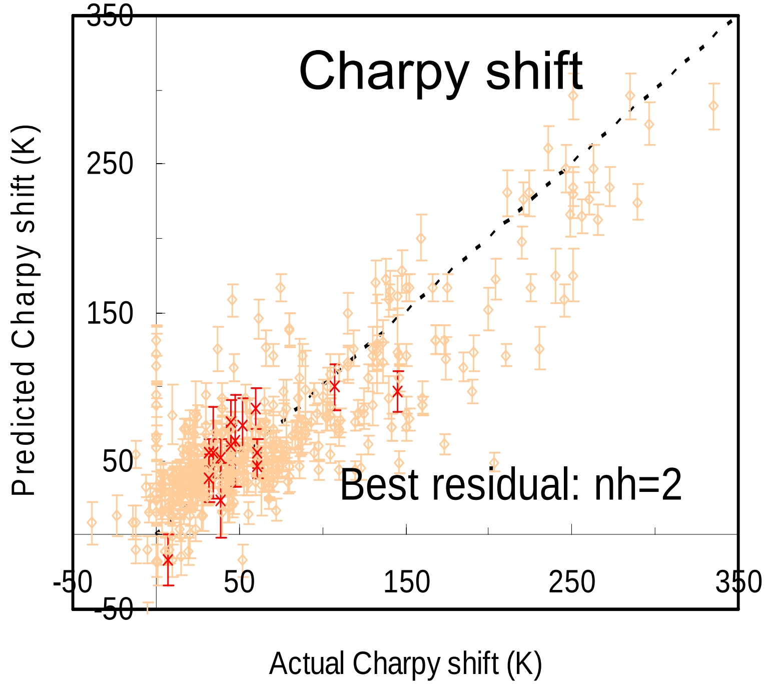
(i) Low hidden unit numbers in neural net fits

(i) Only use inputs which are shown to be beneficial (forward selection of features method)

(iii) Rather than use individual atomic fraction inputs, use linear combinations of inputs (target-driven components method)

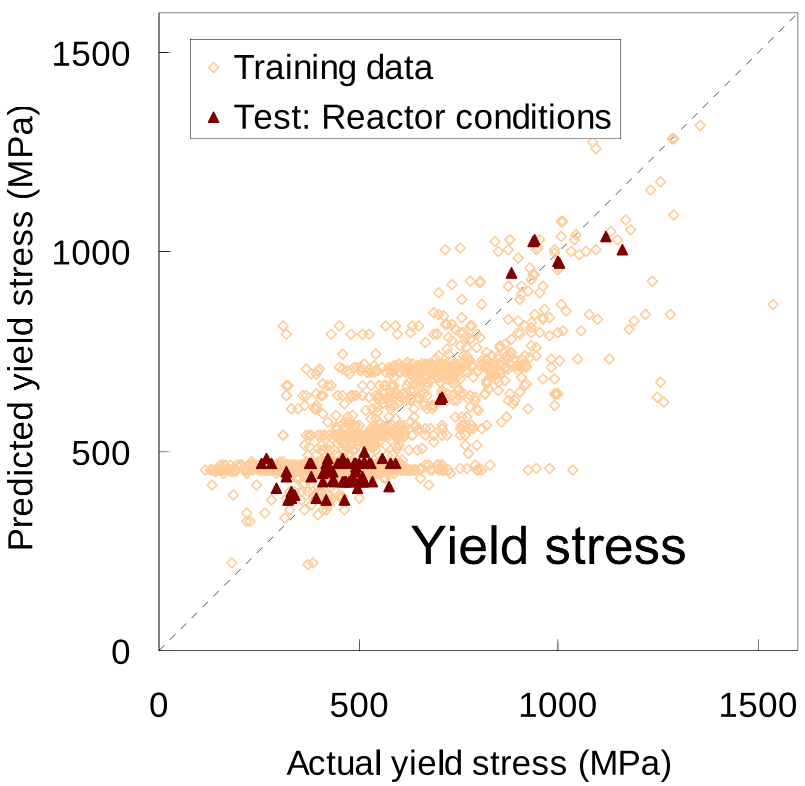
Results with low hidden units

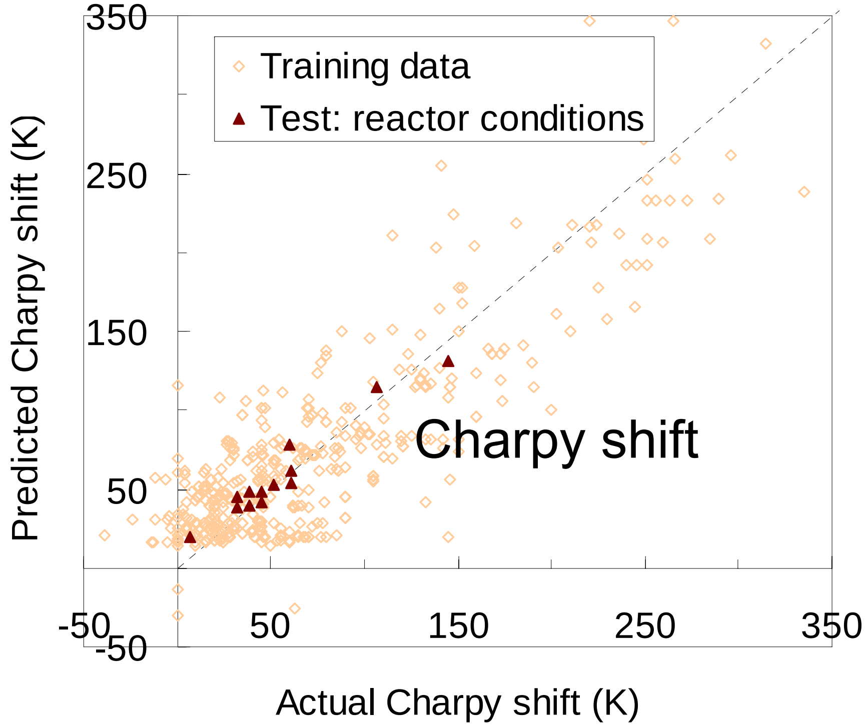




These networks are selected from the previous committee networks to give a optimal fit with the validation data. The validation residual and its error are much improved.

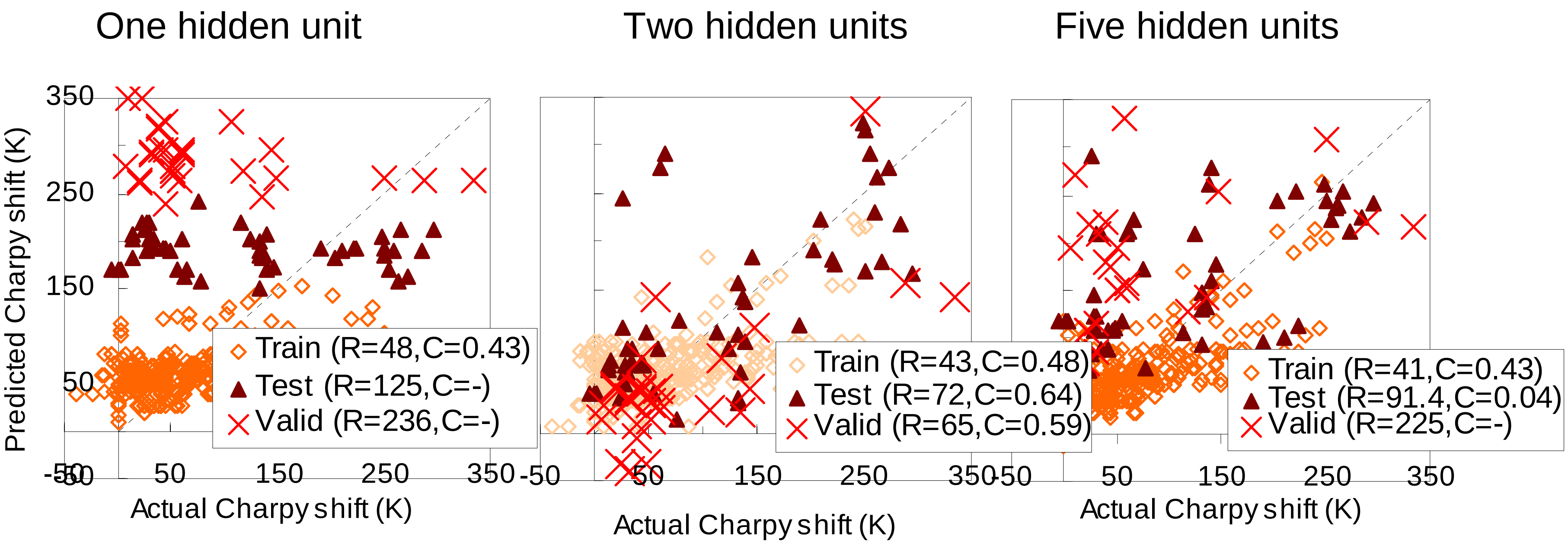
Results with combination inputs





The inputs to these networks are linear combinations of atomic fractions. Performance is even better

Training Charpy data with varying network complexity



The training, testing and validation data scatter plots Charpy shift data. Training data is below 10 dpa, testing data between 10 and 20 dpa and validation data above 20 dpa. The network was trained using atomic concentration inputs.

Finding an optimal alloy

A desirable alloy for a fusion reactor would have:

i) High yield stress: but too high may be brittle
ii) Good toughness – low Charpy shift under irradiation
iii) Low activation after 100 years

We use the neural net to predict the first two properties for each alloy in the database under reactor conditions, and the data of Gilbert and Forrest to predict the activation.

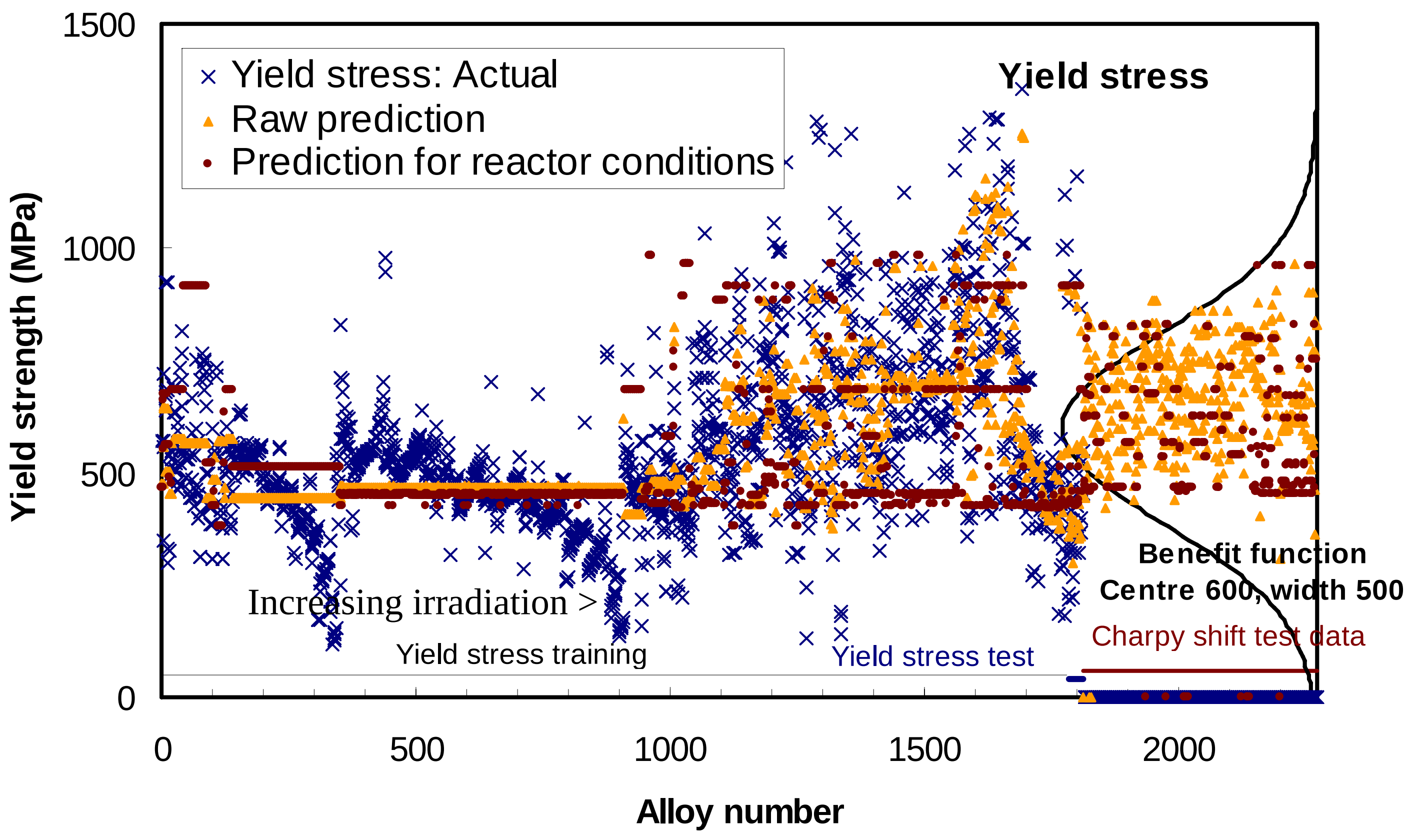
e.g. Irradiation 40 dpa (displacements per atom)
Irradiation temperature 400 C
16 months operation

based on the European Fusion Development Agreement (EFTA) Power Plant Conceptual Study (PPCS model B)

A triple product of "(property value) x (benefit function)" is used to find the optimal series of alloys

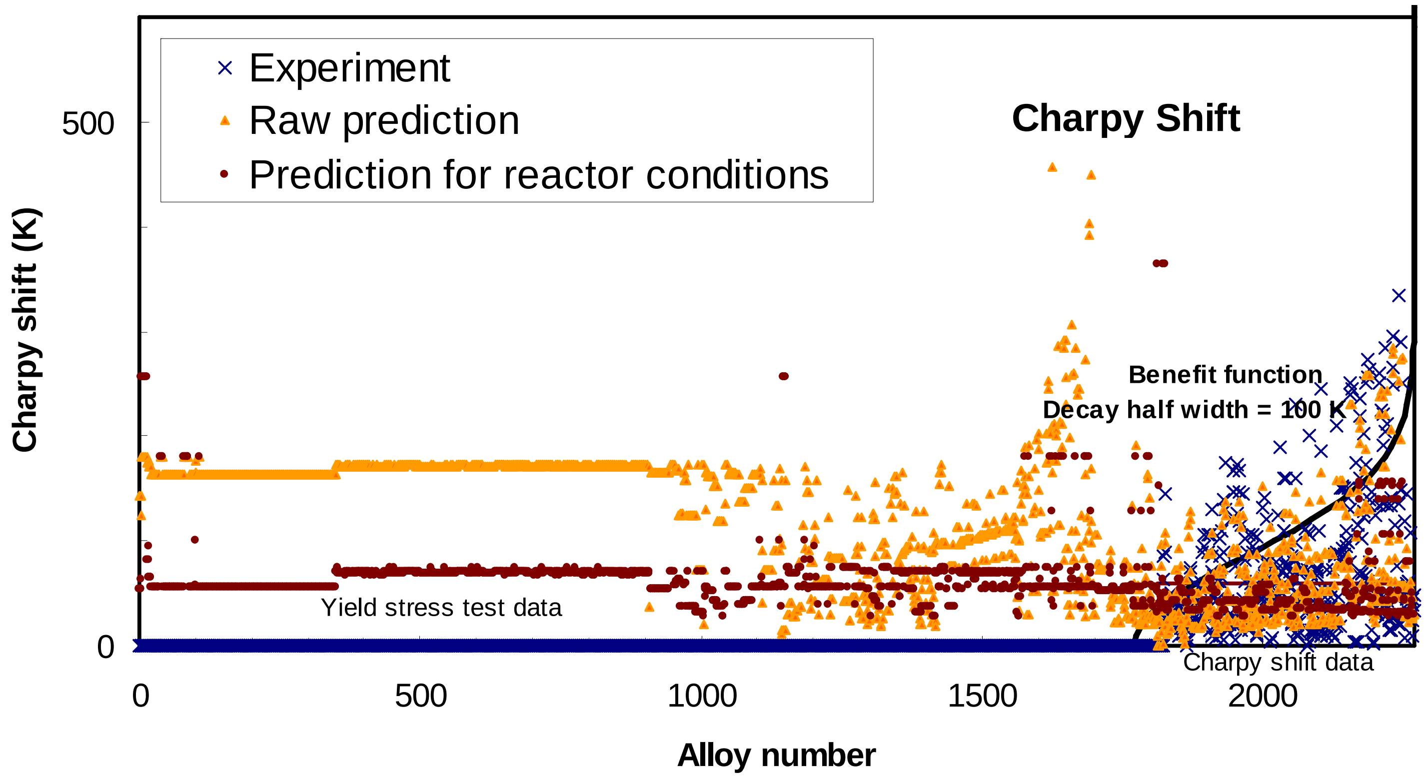
The yield stress of all the alloys

Experimental values are compared with raw predictions for each alloy and with predictions at reactor conditions of 40 dpa and 400 C.



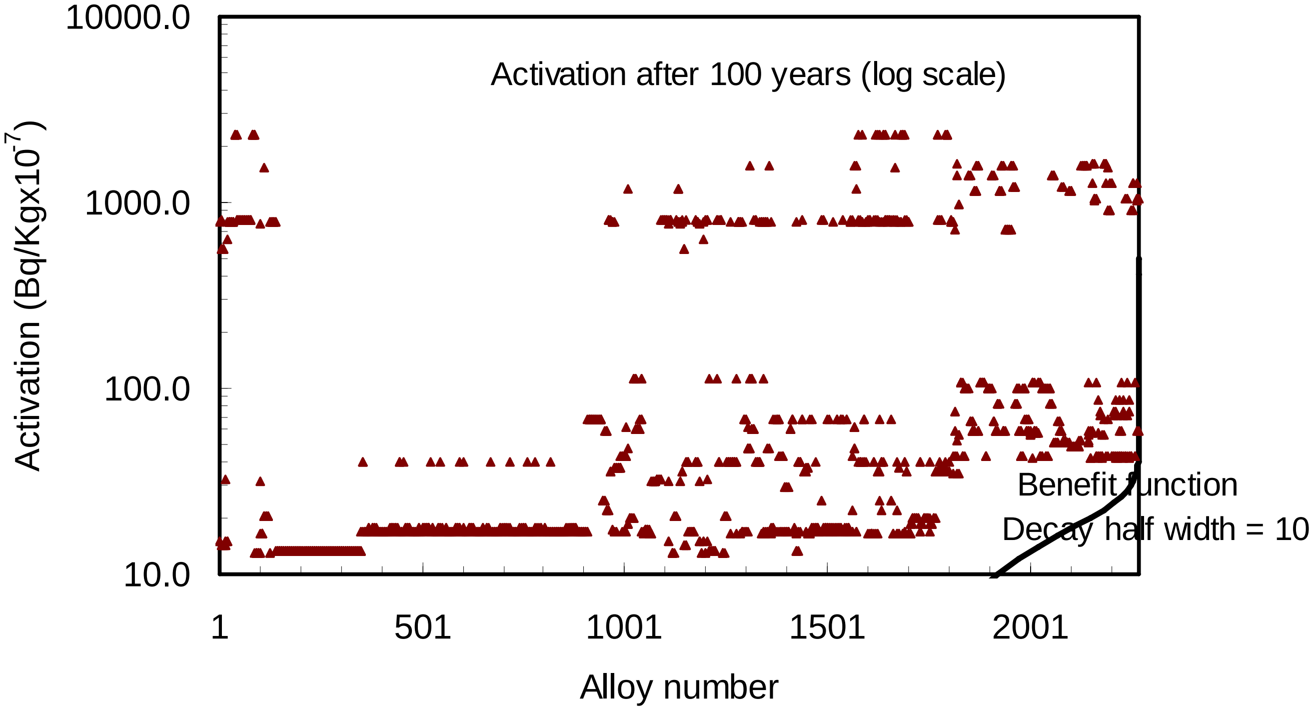
The Charpy shift of all the alloys

Experimental values are compared with raw predictions for each alloy and with predictions at reactor conditions of 40 dpa and 400 C.



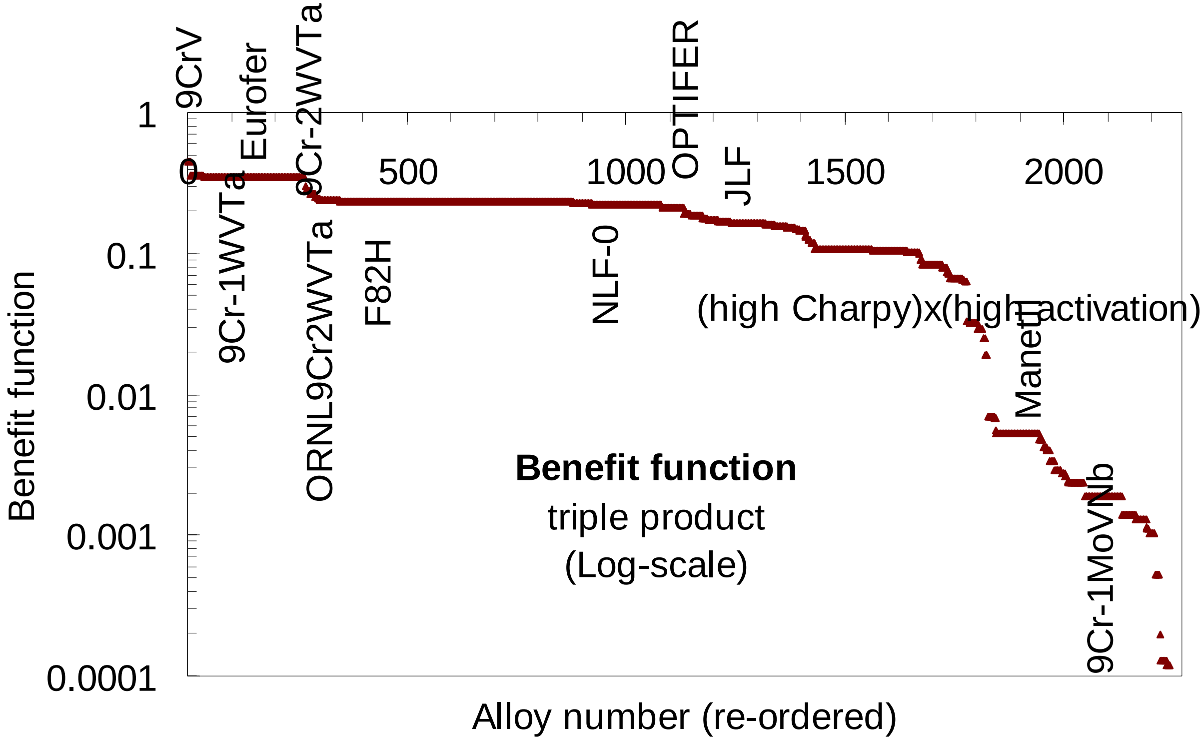
Residual activation after 100 years

Each alloy is assumed to have been irradiated under reactor conditions for 16 months, then left for 100 years (US standard). From Gilbert M R and Forrest R A, 2004



The benefit function: choosing a suitable alloy

Each property (yield stress, Charpy shift and activation) is weighted with the “benefit function” shown by the black lines in the previous three slides and the three products are multiplied together.
The alloys are re-arranged into decreasing benefit order (log scale).



Conclusions

•A fusion reactor has demanding metallurgical problems.
We presently lack reactor-relevant data on irradiated samples

•The yield stress, Charpy shift and activation are important properties for which useful databases exist, especially at lower irradiation levels

•Neural networks can extrapolate these metallurgical properties which appear to vary smoothly with irradiation level and temperature. They therefore provide a framework for predicting reactor-relevant properties

•The alloys within the database have been weighted by a product of "benefit functions" to determine the most suitable of current alloys. These functions can easily be changed.

•The prediction of new alloys using these methods will be the next step