Tensile Properties of Austenitic Stainless Steel

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The choices we make, not the chances we take, determine our destiny.

Preface

This dissertation is submitted for the degree of Master of Philosophy in Materials Modelling at the University of Cambridge. The research described herein was conducted under the supervision of Prof. H. K. D. H. Bhadeshia and Dr. Thomas Sourmail in the Department of Materials Science and Metallurgy, Cambridge, between April 2002 and August 2002. This dissertation contains less than 15,000 words.

Except where acknowledgement and reference is made to previous work, this work is, to the best of my knowledge, original. Neither this, nor any substantially similar dissertation has been, or is being, submitted for any other degree, diploma or other qualification at any other university.

Iqbal Shah.

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Finally, I would like to say how much I love my family. Without their support and encouragement, this year would not have been possible.

Abstract

The short-term mechanical properties of austenitic stainless steels can be affected by a myriad of factors. Materials scientists conduct countless trials to find new steel compositions, in an attempt to optimise the properties. The data are generally analysed using linear regression models [1,2] to reveal more promising compositions. However, they do not envelop the full complexity of the tensile behaviour of steels.

This thesis begins by reviewing the essential factors and hardening mechanisms that affect the mechanical properties of steels. The validity of linear regression analyses is then reviewed and given a critical assessment. As conventional regression methods are not capable of accurately characterising the non-linear trends of steel strength, attention was diverted to neural networks, which can allow for such variations within the data. Neural network models were therefore developed using databases containing composition and other inputs meaningful to steel strength. The ability to calculate error bars, dependent on the location of a prediction within the input space and any perceived noise in the data, is another advantage with this method. Six compositions were chosen to investigate these models. The predicted trends were shown to be in good agreement with the literature and the use of contour plots demonstrated the ability to capture non-linear relationships.

However, it may be desired to reverse the neural network and search for a set of input variables, which result in a desired target output value. This can in principle be done by combining the network with a genetic algorithm. This is a search technique based on the idea of natural selection. Search parameters, such as mutation and crossover, were first investigated to see how convergence to specified target output values could be improved. It was found, as expected, that high numbers of populations, chromosomes and crossovers improved performance. Using these optimal settings, various simulations were conducted, in an attempt to find compositions of a similar tensile strength for austenitic stainless steel. The search process was directed towards a specific output value, but the results showed that the target was not met. Nevertheless, yield strengths of approximately 400 MPa were still predicted. These values were reinforced by the presence of moderate error bars and sensible stainless steel chemical compositions.

Nomenclature

a	Lattice parameter
b	Burgers vector
A	Area
F	Force
T	Temperature
σ	True stress
ε	True strain
K	Strength co-efficient
n	Strain rate sensitivity
τ	Shear stress
L_o	Original length
L	Instantaneous length
ln	Natural logarithm
G	Shear modulus
d_o	Equilibrium stacking fault energy
γ, SFE	Stacking fault energy
ν	Poisson's ratio
f	Equilibrium particle spacing
σ_y, YS	Yield strength or 0.2% proof stress
UTS	Ultimate tensile strength
σ_o	Friction stress
k_y	Grain boundary hardening constant
G_s	Grain size number
fcc	Face centred cubic
t	Annealing twin spacing

σ_w	Model perceived significance
α, β	Hyperparameters in neural networks
M_w	Objective function of neural networks
E_D	Error function in neural networks
E_w	Regularisation term in neural networks
σ_v	Gaussian noise in neural networks

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