Estimation of fracture toughness of tempered nanostructured bainite

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Fine structures consisting of a mixture of extremely thin bainite plates embedded in a matrix of austenite, are now a commercial proposition. Whereas the phase transformation theory for such structures is fairly well established, the understanding of their mechanical properties is not. The present work is an attempt to express the fracture toughness of such steels using a neural network method exploiting data available for martensitic and ordinary bainitic steels. It is demonstrated that in spite of uncertainties, the model captures reasonable trends and is able to estimate unseen experimental results on the nanostructured bainite.

Keywords: Nanostructured bainite, Neural network, Toughness, Modelling

Introduction

There has been a significant progress in the commercialisation[1,2] of the so called nanostructured bainite in which extremely fine, 20–40 nm thick platelets of bainitic ferrite are dispersed in a matrix consisting of carbon enriched retained austenite.[3–5] The latter phase is also in a finely divided state, occupying $\sim$20% of the volume of the steel. The strength of the material, which is often in excess of 2 GPa, is largely due to the fine scale of the structure, which is why only severe tempering leads to significant changes in hardness.[6] However, there is little understanding of the mechanical properties as a function of tempering heat treatments; this applies to bainitic structures in general given that they are in commercial applications largely generated by continuous cooling transformation with no subsequent heat treatment. This can be a severe limitation in attempts at modifying alloys based on the fine structure, for purposes other than those currently in commercial production.

The purpose of the present work was to see if a model based on conventional steels can be exploited to estimate the toughness of nanostructured bainite as a function of heat treatment. The neural network method[7–9] is used to achieve this. There are, however, two difficulties. The first is that there is a lack of appropriate data for tempered bainite. Therefore, the framework that was sought is developed primarily using the much larger quantity of measurements available for tempered martensite. The essential difference between the tempering of martensite and that of bainite is that the former has carbon in solution so that its hardness is more sensitive to heat treatement.[10] There is of course evidence of excess carbon in bainitic ferrite,[11–13] but the concentration is less than that of the parent austenite. Nevertheless, for anything other than tempering at temperatures where only carbon is mobile, or the early stages of tempering, the analogy between the tempering of bainite and martensite should hold. After all, bainite has, since its inception, been regarded as 'being first formed as martensite but is subsequently more or less tempered and succeeds in precipitating carbon'.[14]

The second anomaly in the present work is that the nanostructured bainite does not contain carbides but instead has a substantial quantity of retained austenite. To see whether the work would be able to reasonably estimate the fracture toughness obtained on tempering this mixture, a number of new experiments are reported and specific data for carbide-free bainite available in the literature are tested against the model created. This is described towards the end of the paper.

Neural network model

The data for analysis were collected from more than 100 publications, a comprehensive list of which can be found in Ref. 15. The variables and their general characteristics are listed in Table 1. The set includes a total of 438 experiments where the toughness is reported as a function of 11 variables.

There are some unavoidable complications with the published data, which may or may not contribute to the noise perceived by the model depending on whether the variable affected has a significant influence on the toughness within the context of the compiled data. The decision was made to exclude the sample dimensions and the notch orientation because these variables are not fully reported and their inclusion would severely limit the size of the dataset. It is possible that the dimensions of the sample used in fracture toughness measurements can be legitimately neglected since the K_{IC} reported are all valid measurements, satisfying plane strain conditions during testing. In the cases where the austenitising

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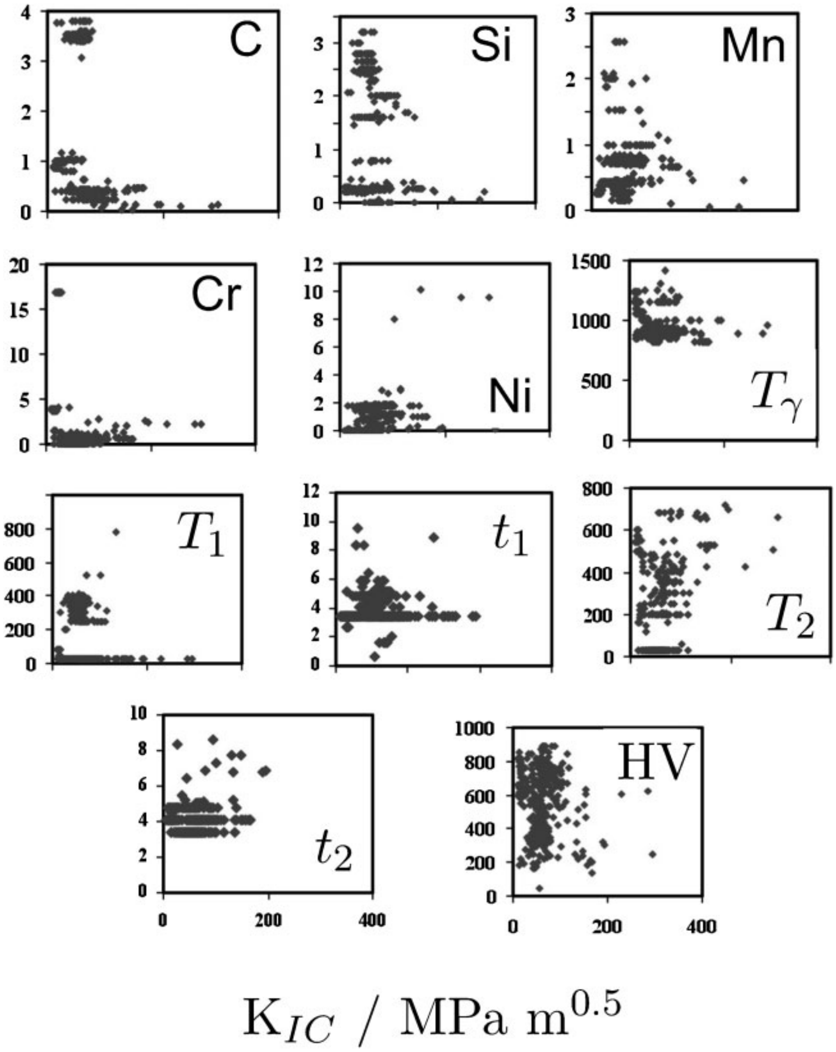


1 Illustration of distribution of data as function of toughness: units on vertical scale of each figure correspond to those in Table 1; horizontal scale in all cases spans from 0 to 400 MPa $m^{0\cdot5}$, with exception of parameter ln t_1 where range is 0–300 MPa $m^{0\cdot5}$

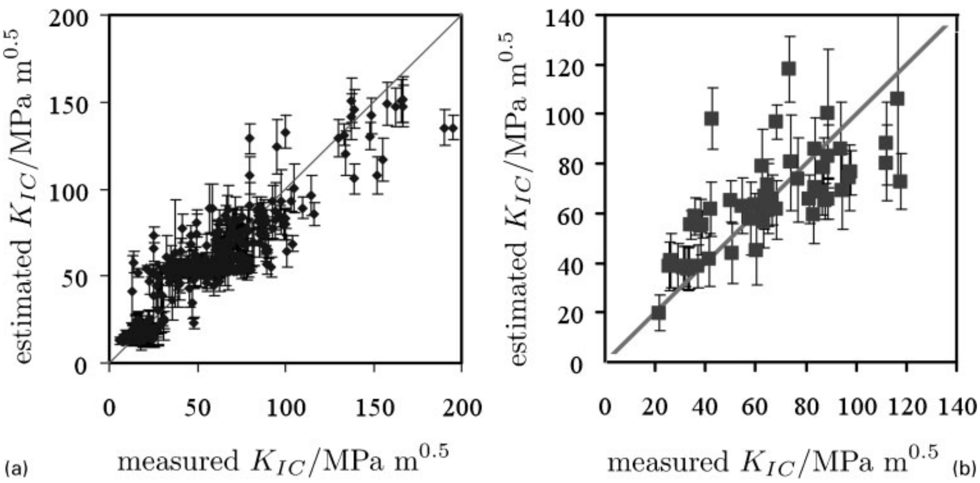
temperature T_γ was missing, it was estimated by calculating the Ae_3 temperature for the steel. In the cases where the hardness value was missing, it was approximated as three times the yield strength[16] when both quantities are expressed in units of kg mm^{-2}. Natural logarithms of the heat treatment times were used as inputs rather than the time itself because the rates of solid state reactions vary logarithmically with time rather than directly, for example, in the classical Avrami theory.

Table 1 Characteristics of data used in creation of model: all toughness values correspond to measurements at ambient temperature

Variable	Min.	Max.	Average	St. Dev.
C/wt-%	0	3·8	1·6	1·4
Si/wt-%	0	3·2	1·3	1·1
Mn/wt-%	0·01	2·6	0·6	0·4
Cr/wt-%	0	16·9	1·5	2·8
Ni/wt-%	0	17·9	1	1·3
T_γ*/°C	816	1423	961	122
T_1/°C	30	780	162	152
t_1/ln (min)	0·69	9·6	3·9	0·95
T_2/°C	20	720	255	223
t_2/ln (min)	3·4	8·6	3·9	0·7
Hardness/HV	93·7	885	455	166
K_{IC}/MPa $m^{0.5}$	5·5	195	55	31

*T_γ is the austenitisation temperature.

The data deal with two possible heat treatment steps at temperatures T_1 and T_2 for time periods t_1 and t_2 respectively, following austenitisation. The first is a direct quench in which case T_1 is set to 30°C and t_1=2 min; the sensitivity of the model to these data is virtually zero given that the parameters have been chosen effectively to indicate no isothermal heat treatment. When the steel is transformed isothermally in step 1, T_1 and t_1 are set to the appropriate values. A subsequent tempering heat treatment defines the values of T_2 and t_2. The distribution of the data as a function of K_{IC} is illustrated in Fig. 1; a large modelling uncertainty is expected when calculations are carried out using the trained model, in regions which are sparsely populated. Modelling uncertainty arises when many different models can reasonably represent the available data, but the models extrapolate differently in domains where data are sparse. This is in contrast to noise, which is a consequence of the neglect of a variable which contributes to the output. Whereas modelling uncertainty



a on data used to create models; *b* on unseen data which were not used to create models, as described in text

2 Illustration of performance of optimum committee of models: error bars represent $\pm 1\sigma$ modelling uncertainty

varies with the position in the input space where a calculation is carried out, the noise is assessed as a constant number over all the data.[7–9,17]

The full details of the neural network method presented here have been described elsewhere,[15] including the search for the optimum committee of models, the procedures used to avoid overfitting the data, and the perceived significance of each input. The constant value of the noise in the output due to unknown variables which are neglected was about $\pm 1\sigma = 8\%$, where σ represents one standard error. The levels of agreement achieved together with error bars representing the modelling uncertainty are shown in Fig. 2; it is evident that the model performs reasonably well not only on the data that were used to create the model, but also on the new data which were collected from the literature.[18–21] It should be noted that these new data are all within the range of input parameters listed in Table 1.

Our main goal was to make predictions on the novel nanostructured bainite described in the introduction, which not only has an unconventional structure, but also falls outside of the range of the model. Some data are available on this structure,[22] but not in the tempered condition; therefore, the next section describes a series of experiments to measure the toughness of the tempered state.

Experimental measurements

The chemical composition of the steel used is listed in Table 2; the alloy has a high carbon concentration with sufficient silicon to prevent the precipitation of cementite during the transformation to bainite. The structure was generated by austenitisation at 1000°C for 1 h, followed by isothermal transformation in a salt bath at 200°C for 9 days. The heat treated samples were in the form of slightly oversized blanks which were then machined to size. Tempering treatments were conducted on the machined samples for the time and temperature combinations listed in Table 2.

X-ray diffraction was used to determine the phase fractions, using Cu K_α irradiation at 40 kV and 40 mA. The sample was scanned over the 2θ range 30–150° and the fractions of ferrite and austenite were calculated using Rietveld analysis[23,24] with the Philips highscore plus software.

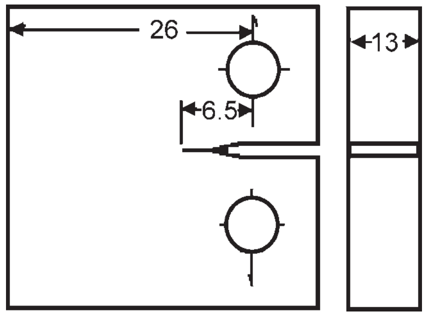
The fracture toughness was measured according to ASTM E399–90 standard[25] using 13 mm thick compact tension specimens (Fig. 3) tested in air at ambient temperature. Fatigue precracks were introduced by sinusoidal loading at 50 Hz on a servohydraulic machine, with a step-down loading method. Hardness measurements were made using a standard Vickers hardness testing machine and are reported in Table 2.

The samples were finish machined after heat treatment in order to avoid effects due to surface degradation. Because it is very expensive to machine the compact tension specimens in the hardened condition of superbainite, only eight of the samples were tested for toughness, and the results are presented in Table 3. It is seen that most of the specimens yield K_Q values because they did not strictly satisfy the criteria for a valid fracture toughness measurement, primarily because the average crack length fell outside of the required range, or because the maximum applied load to the peak fracture toughness load fell outside of the required range. Nevertheless, the values and trends seen are

Table 2 Chemical composition (wt-%) of bainitic steel, together with details of tempering heat treatments: initial Vickers hardness before tempering was 645±8 HV10, and scatter in all of values tabulated below was between ±8 and 12 HV10; temperatures were maintained within ±10°C

C	Si	Mn	P	S	Cr	Ni	V
0·97	1·43	1·59	0·0018	0·0012	0·26	0·04	0·09

Tempering temperature/°C	Tempering time	Hardness/HV10
300	6 h and 1 month	642, 652
400	50, 100, 120, 150, 200, 250, 300, 360, 480 min	632, 637, 625, 628, 626, 625, 625, 611, 612
450	6 h	626
500	6 h	556
600	6 h	377



3 Dimensions of compact tension sample in mm, with diameter of holes being quarter of sample thickness

reasonable and the data were used to compare against the neural network predictions, alongside 10 other data from untempered nanostructured bainitic samples where valid fracture toughness values have been reported.[4,26,27]

The results are presented in Fig. 4 and with one exception, the predictions of the model are reasonable; note that the modelling uncertainty is in all cases quite large, as might be expected since these alloys not only do not fall in the range of the data used in training the model, but also their structures are quite different from normal bainitic steels in the sense that the bainite is free from carbides in spite of their large carbon concentrations. It is notable that tempering actually leads to a reduction in toughness, which contradicts the general experience for martensitic microstructures, but in fact is expected when mixtures of austenite and bainitic ferrite tempered.[28] The retained austenite enhances toughness through transformation plasticity, and tempering causes it to decompose into a mixture of carbides and ferrite.

Conclusions

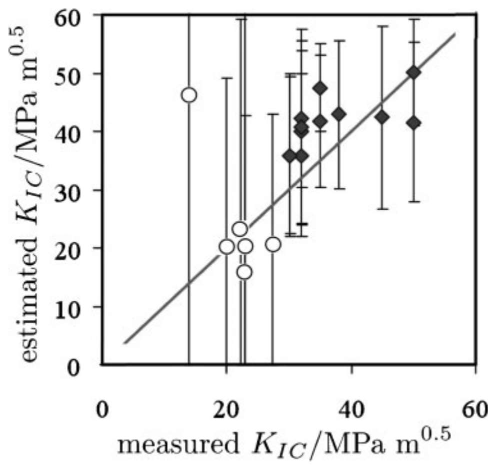
The objective of this work, to develop a model for the fracture toughness of bainitic and martensitic steels in both their virgin and tempered conditions, has been achieved using a neural network method based on published data. Furthermore, the method yields two kinds of uncertainties, the noise and modelling uncertainty, which are useful in assessing the reliability of the predictions made. The aim was to apply this model to a new class of nanostructured, carbide-free bainitic steels for which there is a dearth of data, in the hope that the model can be used in optimising these steels to suit specific applications. It has been demonstrated that although the modelling uncertainties are large when predictions are made on the nanostructured bainite, the trend in the plot of predicted versus measured data is sufficiently reasonable for the model to be useful in future work.

The complete model is freely available on www.msm.cam.ac.uk/map/mapmain.html.

Table 3 Toughness data

Condition	K_Q or K_{IC}/MPa m$^{0.5}$
Untempered sample	31*
Tempered 300°C for 6 h	27*
Tempered 300°C for 1 month	23*
Tempered 400°C for 8 h	23
Tempered 450°C for 6 h	20*
Tempered 500°C for 6 h	22*
Tempered 600°C for 6 h	14*

*K_Q values, i.e. not strictly valid in terms of the ASTM standard.



4 Comparison of measured fracture toughness of superbainite both in isothermally transformed (solid points) and tempered (unfilled circles) conditions, against model estimates: error bars represent $\pm 1\sigma$ modelling uncertainty and it is emphasised that some of values plotted are K_Q data as explained in Table 3

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