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A Model for The Prediction of Fracture Toughness Using Neural Network

Dr. Aseel abdulbaky
Electromechanical Engineering Department, University of Technology/Baghdad
Email:aseelbaky@yahoo.com
Dr. Dhafer Al-Fattal
Mechanical Engineering Department, University of Technology/Baghdad
Dr. Harry Bhadeshia
Material Science and Metallurgy Department, University of Cambridge/UK.
Dr. Talal Abdul Jabbar
Electromechanical Engineering Department, University of Technology/Baghdad

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ABSTRACT

The purpose of this research programme is to develop quantitative models for the prediction of mechanical properties (fracture toughness) using experimental data collected from the literature, together with a powerful computational technique known as neural network. Creating a truly general model requires a combination of available data and metallurgical knowledge.

This model is proposed for martensitic and ordinary bainitic steels in addition to the more recent class of non-structural super-bainitic steels. Super-bainitic steels are attractive for many applications such as armour. The model of fracture toughness, based on chemical composition, heat treatment an

d mechanical properties is proposed.

The predictions of fracture toughness are generally acceptable but the uncertainties are high and more input data need to be collected for super-bainitic steels when available in the future to improve the predictions of this model.

Keywords: fracture toughness, predictions, neural network.

نموذج لتنبؤ متانة الكسر باستخدام الشبكة العصبية

الخلاصة

يهدف هذا البحث الى التوصل الى نماذج كمية للتنبؤ بالخواص الميكانيكية (متانة الكسر) باستخدام بيانات عملية تم جمعها من بحوث سابقة ، واعتماد طريقة حسابية رصينة تعرف بالشبكة العصبية . ان استحداث نموذج عام يتطلب في الحقيقة بيانات متوفرة ومعروفة بعلم المعادن وتصلح النماذج المقترحة للصلب المارتنسيتي والصلب البينايتي العادي ، اضافة الى الصنف الحديث من الصلب البينايتي الفائق الجودة والذي يعتبر مناسبا لكثير من التطبيقات الهندسية كدروع المركبات العسكرية . تم اقتراح نموذج خاص بمتانة الكسر بالاعتماد على التركيب الكيماوي والمعاملة الحرارية والخواص الميكانيكية في بنائه وكانت تنبؤات النموذج المحسن مقبولة عامة ولكن مدى تذبذب النتائج كان كبيرا. لتحسين تنبؤات هذا النموذج يجب تجميع بيانات جديدة خاصة بالصلب البيانايتي الفائق الجودة عندما تصبح متوفرة.

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2412-0758/University of Technology-Iraq, Baghdad, Iraq

INTRODUCTION

Fracture toughness is an indication of the amount of stress intensity, *K*, required to propagate a pre-existing flaw. It is an important material property since the occurrence of flaws is not completely avoidable in the processing, fabrication, or service of a material or component. Flaws may appear as cracks, voids, metallurgical inclusions, weld defects, design discontinuities, or some combination therefore. Since engineers can never be totally ensure that a material is flaw free, it is a common practice to assume that a flaw of some chosen size will be present in components and linear elastic fracture mechanics (LEFM) approach is used to design critical components. The minimum value of the streets intensity factor, which occurs under plane strain conditions, is designated K_{1c} [1].

K_{1c} is a basic material property and it is strongly dependent on such metallurgical variables as heat treatment, texture, melting practice, chemical composition, impurities, etc.[1].

Creating a model using neural network method requires a large amount of data and it is sometimes not possible to accomplish easily [2]. Creating a truly general model requires a combination of data and metallurgical knowledge [3]. In building the model, the intention of this investigation was to include data for super-bainite steels in addition to the ordinary bainitic and martensitic steels. Super-bainitic steels have found application in armour because of their ballistic properties [4,5]. Many models have been developed in recent years and have been briefly described in [6].

The aim of this paper is to predict the plane strain fracture toughness; the data have been collected from published literature. Different types of steels and austempered ductile irons have been included in these data to create the model. In this work, neural network is used to model the plane strain fracture toughness as a function of chemical composition, transformation temperature, including isothermal transformation and direct quenching, tempering for wide range of steels and mechanical properties (yield stress and hardness). The design of the model is described and to test its validity, prediction is compared with experimental values and expectations.

EXPERIMENTAL PROCEDURE

Material

A high carbon low alloy steel has been used in the experimental tests to validate the model of plane strain fracture toughness. The chemical composition of this alloy is shown in Table (1). The material was made in the form of 50 kg ingot by vacuum induction melting [7].

Table (1) Chemical composition of alloy wt % [7].

C	Si	Mn	P	S	Cr	Ni	V
0.97	1.43	1.59	0.0018	0.0012	0.26	0.04	0.09

FURNACE HEAT TREATMENTS

The as received material was austenitised at 1000°C for one hour in a salt bath and then isothermally transformed at 200°C using a salt pot for 9 days. The samples were then oil quenched to room temperature. All the samples were as blanks, and the final notch was machined after the heat treatment. Some of the samples were tempered at different temperatures and different times as listed in table 2.

Table (2) The values of tempering temperature and tempering time on the alloy.

Tempering Temperature °C	Tempering time
300	6 hours and 1 month
400	(50, 100, 150, 200, 250, 300) minutes and (2, 6 and 8) hours
450	6 hours
500	6 hours
600	6 hours

Plane strain fracture toughness tests

The fracture toughness test was conducted according to ASTM E 399-90 standard [1] in order to obtain the plane strain fracture toughness K_{1c} of the material. Compact tension specimens were machined from the blanks. One sample was used for each tempering temperature, and the test was conducted in laboratory air at ambient temperature.

The samples were tested on two different machines, the first machine was Mayes 100 kN Servo Hydraulic Machine, to fatigue pre-crack the sample using a sine wave loading with a frequency of (50 Hz). A step-down loading method was used during fatigue pre-cracking. After the pre-crack has reached the required length, the sample was removed and prepared for the fracture toughness test.

The second machine was an LCF tester with a maximum load capacity of (100 kN). The sample was loaded with a very slow loading rate of 1 mm/min. The load-displacement was digitally recorded by a computer and the Bluehill®2 Software was used for data output.

THE EXPERIMENTAL RESULTS

This work studied the effect of tempering for different times and temperatures on the stability of the microstructure and mechanical properties in this alloy.

XRD test results

X–ray diffraction was used to determine the phase fractions, using *Cu Ka* irradiation at 40 kV and 40mA. The sample was scanned over the 2θ range 30–150◦ and the fractions of ferrite and austenite was calculated using the Philips Highscore–plus software.

The volume fraction of the phases in the alloy were measured in the as-transformed condition and after tempering using X–ray diffraction as shown in fig. 1, and table 3. It can be stated that the volume fraction of retained austenite decreases with the increase of the tempering temperature. It is speculated that a small amount of austenite will still be present in the structure until the tempering temperature reaches 500 °C, but will completely decompose just below 550 °C which leads to a change in thickness of the bainite plates as was explained in [8].

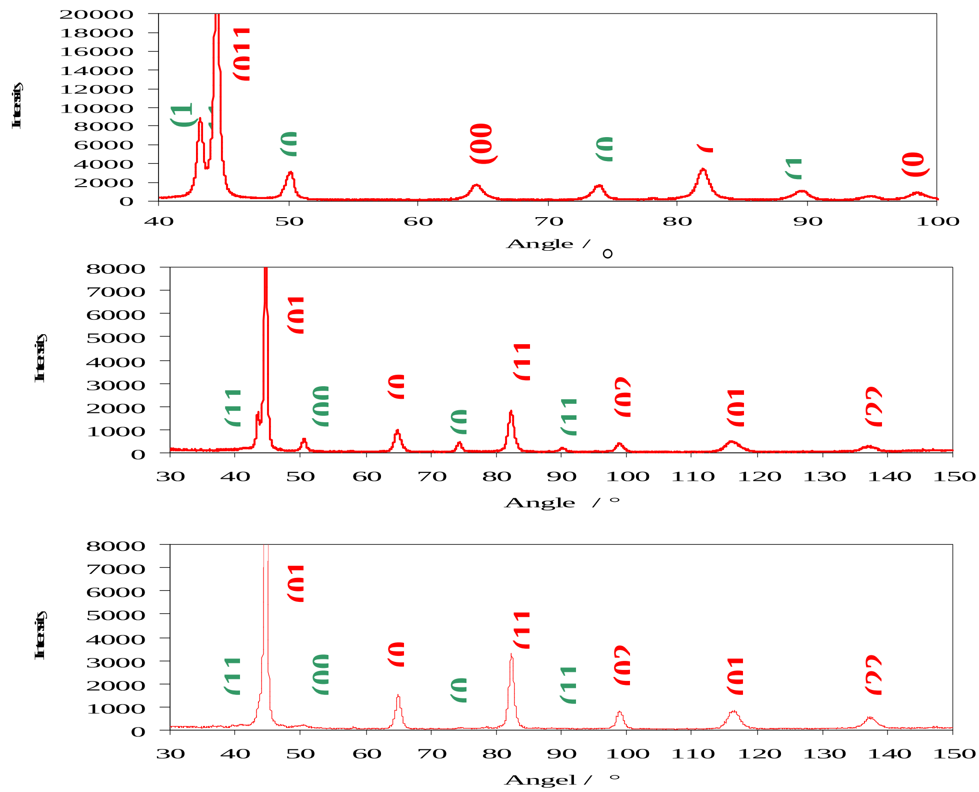


Figure (1) The XRD of material, (a) as transformed, (b) after tempering at 400 °C for 6 h (c) after tempering at 450 °C for 6 h

Table (3) Result of X-ray diffraction analysis.

Condition	Austenite (volume percent)	Lattice Parameter (for austenite/ Å)	Ferrite (volume percent)
As transformed	32±0.000113	3.6265±0.000084	67.9±0.000736
Tempered at 400 °C for 6h	15.5 ± 0.4	3.60743 ± 0.0004	84.52 ± 0.4
Tempered at 450 °C for 6h	4.5 ± 0.55	3.5988 ± 0.0056	95.48 ± 0.55

Tensile properties

The tensile properties were determined from stress-strain traces from standard tensile tests. The yield and ultimate tensile strength of the alloy in the isothermally hardened condition were 1383 MPa and 1622 MPa respectively. The results of tensile tests for the alloy after tempering at different temperatures are shown in Table 4. The mechanical properties did not greatly change with different tempering temperatures. The sample tempered at 400 °C gave an unreliable value possibly due to presence of defects or inclusions in the sample.

Table (4) The values of yield strength (sy) and ultimate tensile strength (su) for the samples tempered at different tempering conditions.

Sample Condition	s_y / MPa	s_u / MPa
Isothermally hardened	1383	1622
Tempered at 300 °C for 6 hours	1285	1285
Tempered at 400 °C for 8 hours	950	968
Tempered at 450 °C for 6 hours	1253	1289
Tempered at 606 °C for 6 hours	1267	1514

Fracture toughness

The reported plane strain fracture toughness value is 30 MPa m0.5 for the isothermally transformed material. In this work, K_Q was found to be 31.18 MPa m0.5 as shown in table 5 which is close to the standard value.

Table 5 lists the K_Q values for these tempering conditions and the validity of the plane strain fracture toughness tests in this table ac the average crack length does not satisfy the standard requirements, P_{max} maximum applied load, P_Q the fracture toughness load and P_f the maximum fatigue load. The general trend is a decrease in fracture toughness as the tempering temperature increases. This is related to the microstructure of this alloy. As it was explained in [9], this is consistent with grain growth when it starts to occur and is not chiefly dependent upon carbon in solid solution.

Table (5) The values of KQ for the samples tempered at different tempering conditions on the alloy.

Sample Condition	KQ (MPa m0.5)	Status	Reason
Isothermally hardened	31	Not valid	*ac* out of the range
Tempered at 300 °C for 6 hours	27	Not valid	$P_{max}/P_Q > 1.1$
Tempered at 300 °C for 1 month	23	Not valid	ac less than the range
Tempered at 400 °C for 8 hours	23	Valid	-
Tempered at 450 °C for 6 hours	20	Not valid	*ac* less than the range
Tempered at 500 °C for 6 hours	22	Valid	-
Tempered at 606 °C for 6 hours	13.8	Not valid	$P_f / P_Q > 0.6$

THE MODEL OF THE FRACTURE TOUGHNESS

Plane strain fracture toughness database

Many attempts were made to build the best model capable of estimating the value of KIc correctly. Three general models have been created which depend on the choice of input variables. These models are:

1- Mechanical properties model.

2- Chemical composition model.

3- Chemical composition, heat treatment and mechanical properties model.

Since the KIc is a function of many variables, the choice of the inputs for the third model is as follows:

$$K_{Ic} = f\,(C_i, T_a, T_{t1}, t_{t1}, T_{t2}, t_{t2}, M_p) \qquad (1)$$

where C_i is the chemical composition (carbon, manganese, silicon, chromium, nickel and molybdenum), Ta the austenitisation temperature °C, T_{1t} the transformation temperature °C, tt1 the hold time at temperature in minutes , T_{t2} the second step temperature °C, t_{t2} the hold time for the second step temperature in minutes and Mp mechanical properties (yield, and hardness).

A dataset consisting of 443 experiments was compiled including sixteen variables. The decision was made to exclude the dimensions of the test sample, the orientation of the notch and the loading direction of the sample. This may add noise to the calculation of toughness but including these variables would limit the size of the dataset. When the austenitizing temperature was missing in the data, it was estimated from other data with approximately similar carbon content or from the *Ae3* temperature for that steel. When either the hardness or yield strength was a missing, it was estimated from the relationship $sy=h/3$. Hardness values in Rockwell and Brinell were converted to Vickers hardness before being fed to the data [8]. The minimum and maximum values for each variable are presented in table 6.

Some of the experimental results explained in this work were added as new data points. These new data points included four values for fracture toughness values for tempered nanostructure bainite in the alloy. All the data which were collected from literature represents tests carried out at room temperature.

Table (6) Data used in the chemical composition, heat treatment and mechanical properties model.

Variables	Minimum	Maximum	Average	St. Dev
C / wt%	0.040	3.81	1.52	1.43
Si / wt%	0	3.21	1.33	1.10
Mn / wt%	0.04	2.58	0.63	0.42
P / wt%	0	0.48	0.015	0.02
S / wt%	0	0.46	0.03	0.102
Mg / wt%	0	1.25	0.07	0.21
Cu / wt%	0	1.60	0.183	0.31
Cr / wt. %	0	16.91	1.28	2.94
Ni / wt%	0	10.06	1.157	1.21
Austenitisation temp. / °C	816	1423	936	104
Temperature step 1 / °C	30	780	161	150
Time step 1 / min	2	14400	137	812
Temperature. Step 2 / °C	28	720	226	205
Time step 2 / min	30	5400	112	402
Yield stress / MPa	236	2300	1174	388
Hardness / HV	48.96	889	547	188
K_{Ic} / MPa $m^{0.5}$	9.8	295	62.7	35

Models training

The data in table 6 was trained and tested. The training and testing method is explained elsewhere [2,3]. Training and testing have shown that both of mechanical properties and chemical composition models have large scatter and noise. Predictions were made using these committees for the chemical composition, heat treatment and mechanical properties. A total of 100 networks were trained by half of the data and tested with another half. The complexity is shown in fig. 2a. The test error has a minimum value at about nine hidden units, fig. 2b. The LPE displays a high degree of scatter; with a rough peak in eight hidden units, fig. 2c. More reliable results were obtained by combining models into a committee. In this case, the optimum committee was found to have fifteen sub models, fig. 2d with the minimum test error.

Fig. 3 shows prediction of the modified model for the entire data. Fig. 4 shows the neural network perceived significance, s_w, for each input variable. In particular, note the committee opinions on the significance of carbon, copper, silicon, manganese and nickel. For heat treatment, temperature and time of tempering and austenitizing temperature have high significance and the hardness has higher significance than the yield stress.

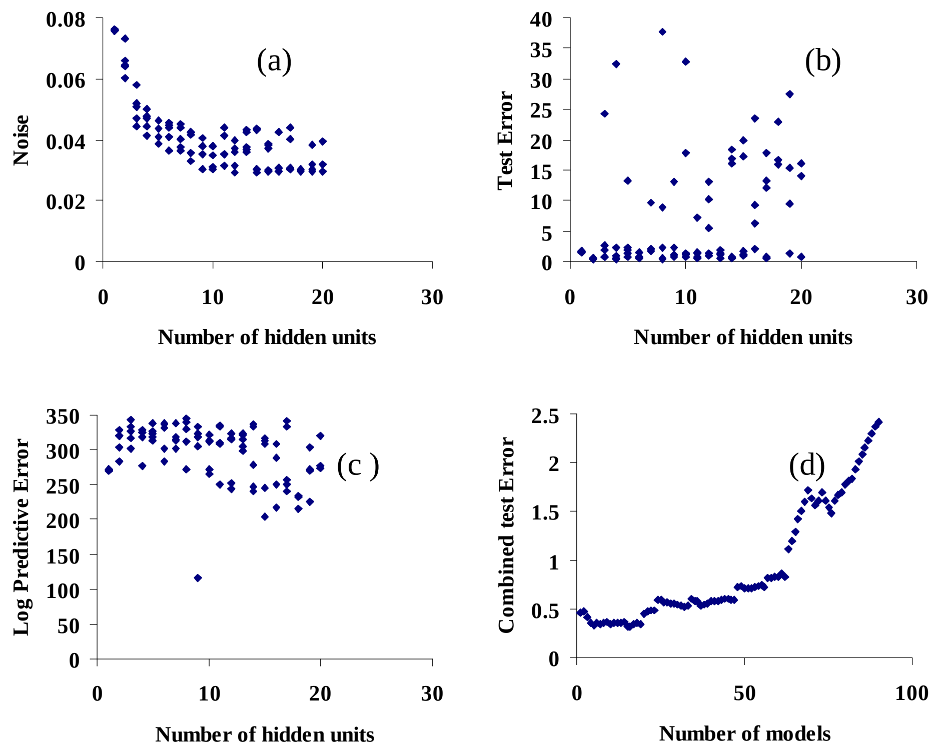


Figure (2) Optimum model training reports: (a) Perceived level of noise for training, (b) the error between the models and the test data, (c) log predictive error for increasing model complexity, (d) combined test error for different sizes of committee.

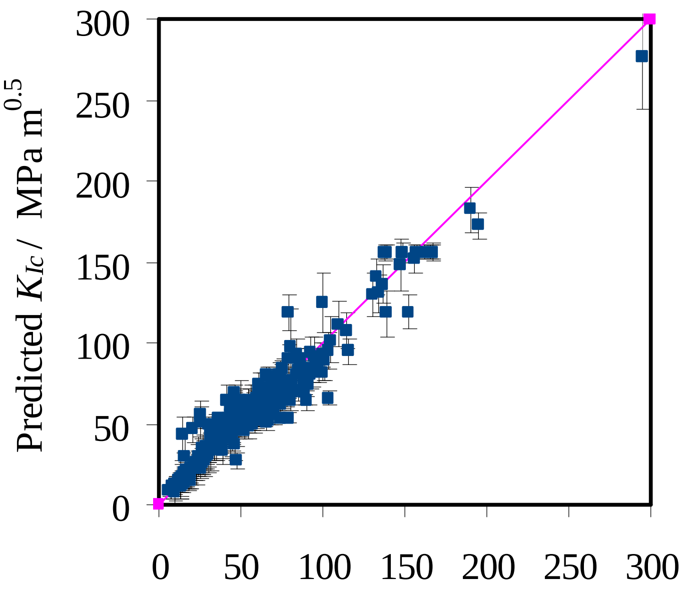


Figure (3) Predictions by the committee model for the entire dataset for the chemical composition, heat treatment and mechanical properties optimized model.

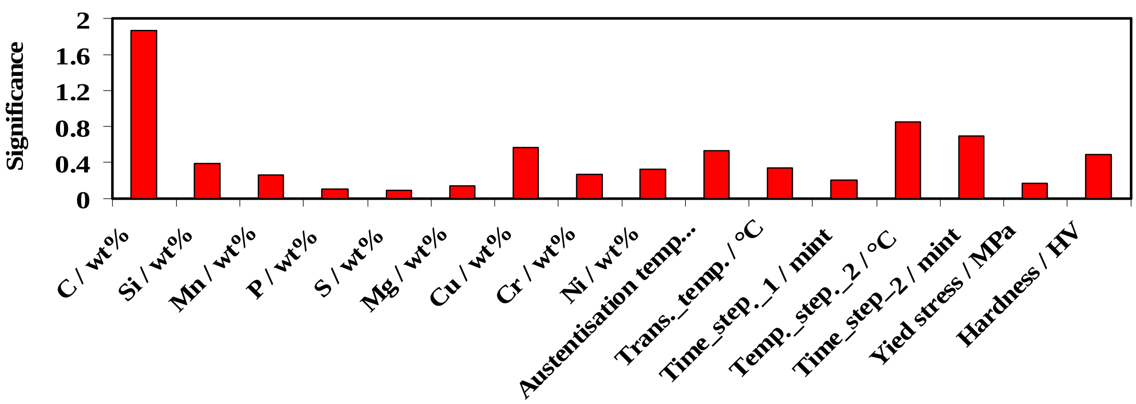


Figure (4) Perceived significance for the committee of the optimized model.

Model predictions

The toughness of steels depends on many variables as stated before. Therefore, it is not possible to predict the plane strain fracture toughness with any reliability.

The input compositions for all the predictions were made with (0.98C- 1.46Si-1.89Mn-1.26Cr wt%), austenitisation temperature 1000 °C, transformation temperature to bainite 200 °C for ten days. All the information about this alloy is found in [9]. Estimates were not made for all alloys in the database.

3.1 Effect of chemical composition on fracture toughness

The effect of carbon content on KIc was explained previously and is shown in fig 5. The trend is an increase in KIc with increasing carbon content. There is a change in error bars, starting with a relatively high error bar at about 0.5 wt% carbon content and then decreasing to a minimum at about 0.9 wt% carbon content and then increasing again up to 1.2 wt% carbon content. From iron carbon equilibrium phase diagram, carbon dissolve completely in the austenite phase between 0.6-1.5 wt% carbon content at 1000 °C and the increase of carbon content in the austenite phase increases the stability of that phase [10]. The volume fraction of bainite, is calculated according to eq.2

$$V_b = \frac{x_{T_0'} - \bar{x}}{x_{T_0'} - x_{a_b}} \qquad \text{…..(2)}$$

where V_b the volume fraction of bainite, $x_{T_0'}$ the austenite carbon content given by the T_0' boundary (the boundary at which the α and γ have the same free energy at a specified temperature)[11], $\bar{x}$ is the alloy average carbon concentration and x_{a_b} is the carbon concentration of the bainite [11].

The V_b will decrease with increasing carbon content and the volume fraction of the austenite stable phase will increase. This austenite is supposed to be a tough phase. After 1.2 carbon content, the toughness might decrease because the brittle cementite phase will appear with austenite. In the region between 1-1.2 C wt%, the prediction shows high error bars and sparse and noisy data that give an indication of a probable drop in toughness.

Fig ure(6) shows the effect of silicon on the K_{Ic}. The K_{Ic} increases with an increase in the silicon content from approximately 0.6 to 2.6 wt%. Silicon hinders the formation of the cementite phase, leading to an increase in KIc with increasing silicon content [11]. Silicon is a ferrite stabilizer; it slows the kinetics of transformation to bainite [10] which means more tough austenite will form.

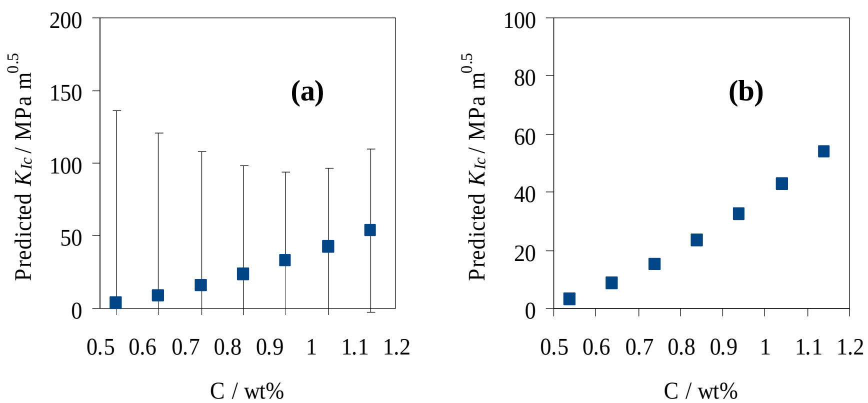


Figure (5) Predictions of plane strain fracture toughness in MPa $m^{0.5}$ against carbon content in wt%, (a) with error bars, (b) general trend.

Figure (7) shows that KIc decreases as the chromium content increases. Chromium leads to solid solution hardening which may make the ferrite more stable than the austenite. The error bars look almost constant, i.e. they come from an uncontrolled variables noise.

Figure (8) shows that KIc has a minimum value at a copper content of 1 wt%. Figure (9) shows that the minimum value of KIc is at a nickel content of about 2 wt%. These two elements may not influence much the microstructure and the toughness of super bainite.

In general, alloying elements (except carbon) do not affect the plane strain fracture toughness that much and only the carbon content has a significant effect.

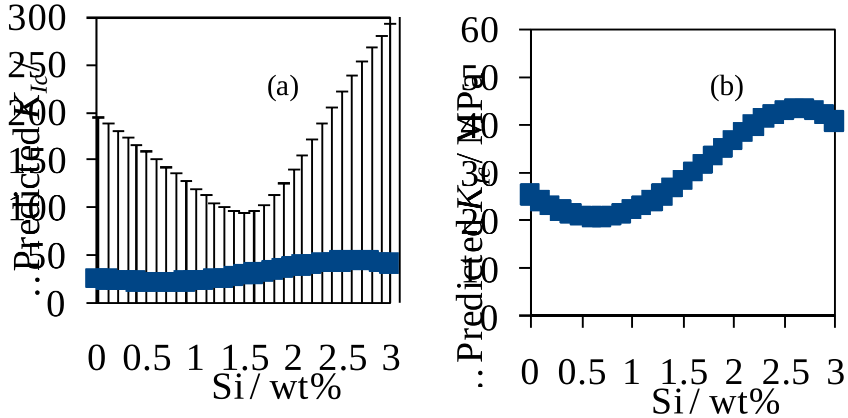


Figure (6) Predictions of plane strain fracture toughness in MPa m$^{0.5}$ against silicon content in wt%, (a) with error bars, (b) general trend.

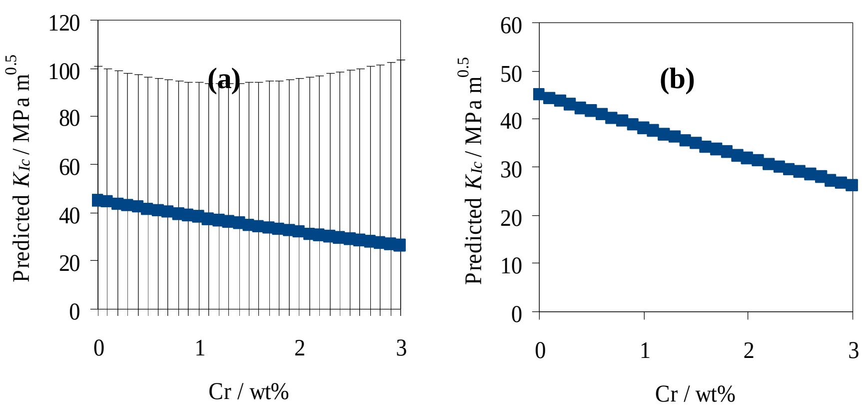


Figure (7) Predictions of plane strain fracture toughness in MPa m$^{0.5}$ against silicon content in wt%, (a) with error bars, (b) general trend.

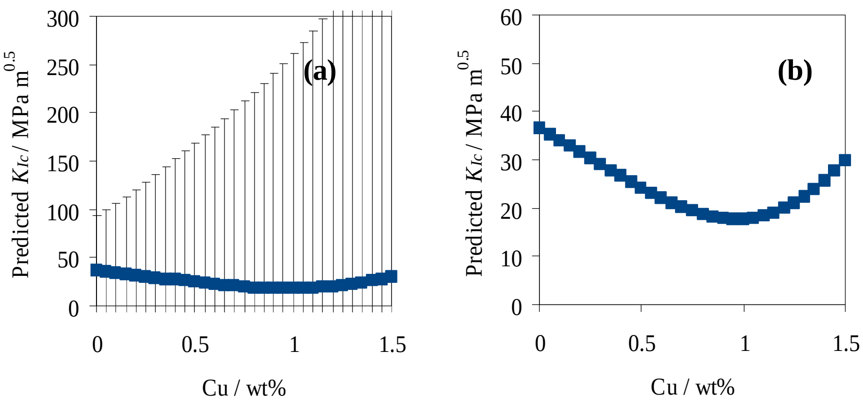
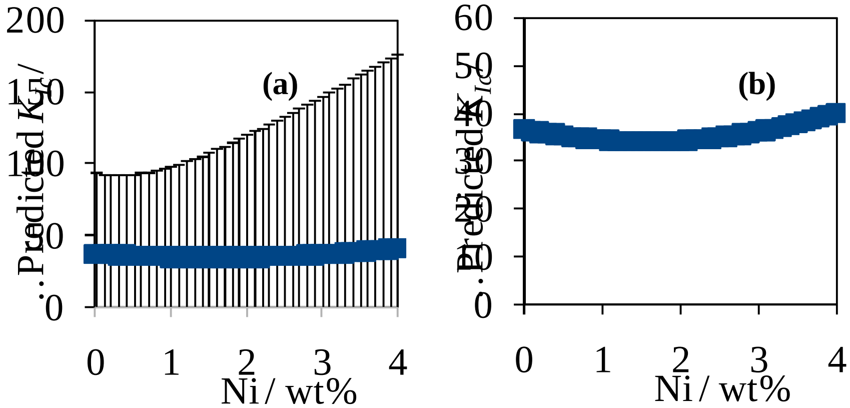


Figure (8) Predictions of plane strain fracture toughness in MPa m$^{0.5}$ against copper content in wt%, (a) with error bars, (b) general trend.



Figure(9) Predictions of plane strain fracture toughness in MPa m$^{0.5}$ against nickel content in wt%, (a) with error bars, (b) general trend.

Effect of mechanical properties on plane strain fracture toughness

Fig. 10 shows a decrease in KIc with an increase in hardness.

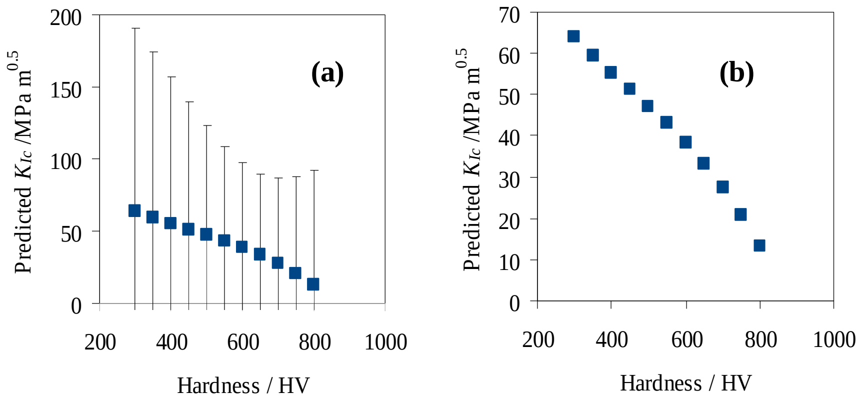


Figure (10) Predictions of plane strain fracture toughness in MPa $m^{0.5}$ against Vicker hardness in committee, (a) with error bars, (b) general trend.

PREDICTIVE ABILITY

The general performance of the model can be tested by predicting on unseen data. These were grouped into those within the range of data used for training and those outside the range.

The general performance of the model can be tested by predicting on unseen data. Fig. 11 shows the predicted plane strain fracture toughness against the actual values [12,13, 14, 15]. Other data concerning alloys with super bainite was collected and tested by the model. Fig. 12 shows the relation between the predicted and measured values.

Table 7 shows the perceived error of the models, and the root mean squared error, to compare the performances of the model. The model fracture toughness has the least difference between the perceived error and the root mean squared error

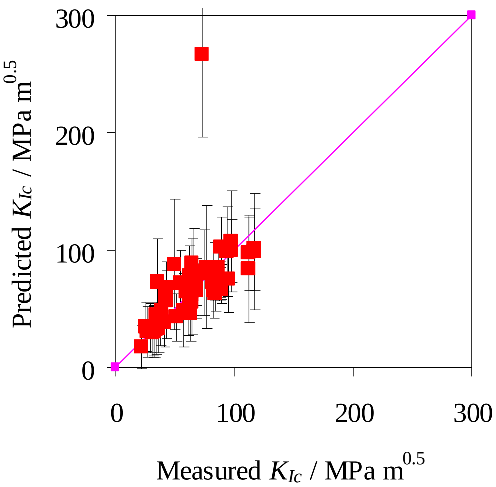


Figure (11) Predictions of plane strain fracture toughness in MPa m0.5 against the measured plane strain fracture toughness in MPa m0.5 for the model of chemical composition, heat treatment and mechanical properties.

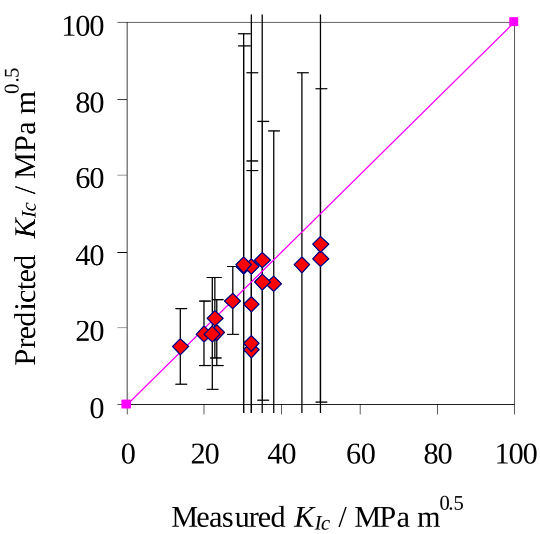


Figure (12) Predictions of plane strain fracture toughness in MPa m0.5 against the measured plane strain fracture toughness in MPa m$^{0.5}$ for the model, the measured values are for the alloy in this work and other alloys from references [8, 16, 17] .

Table (7) The performance of the model is in terms of the root mean square and perceived error.

The modified model	Root mean squared error	Perceived error
For unseen data	29	25

CONCLUSIONS

The main conclusions of this investigation are:

1. A neural network model based on chemical composition, heat treatment and mechanical properties has been proposed to predict the fracture toughness of steels.
2. The model can be applied to super-bainite steels. In general, the predictions are acceptable but the modeling uncertainty tends to be large.
3. More input data need to be collected for bainitic steels as more research is published in the future to improve the predictions of the model.

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