

Prediction of fracture toughness temperature dependence from tensile test parameters

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Abstract

The reference temperature localizing the fracture toughness temperature diagram on temperature axis was predicted based on tensile test data. Regularization neural network was developed to solve the correlation of these properties. Three-point bend specimens were applied to determine fracture toughness. The fracture toughness transition dependence was quantified by means of master curve concept enabling to represent it using one parameter, i.e. reference temperature. The reference temperature was calculated applying the multi-temperature method. Different strength and deformation characteristics and parameters were determined from standard tensile specimens focusing on data from localized deformation during specimen necking. Tensile samples with circumferential notch were also examined. In total 29 data sets from low-alloy steels were applied for the analyses. A good correlation of predicted and experimentally determined values of reference temperature was found.

Key words: steels, brittle to ductile transition, fracture, toughness, artificial neural network (ANN)

1. Introduction

The master curve concept is rapidly becoming an essential part of the evaluation of brittle fracture behaviour of low-alloy steels in various structural applications. This is especially visible in the evaluation of changes in transition behaviour of steels caused by changes of microstructural state, e.g. by the operational degradation of steels. The master curve concept is based [1] on the finding that most ferritic steels with yield strength up to 750 MPa are characterized by the same shape of the fracture toughness transition curve, including the scatter band. The transition behaviour characterizing the particular steel is then defined by the position of this transition curve on the temperature axis. A reference temperature T_0 is used for the positioning the transition region [1, 2]. It is a temperature corresponding to the median value of the frac-

ture toughness equal to $100 \text{ MPa m}^{1/2}$. The concept can be applied in cases when fracture behaviour is controlled by the weakest link and fracture toughness characteristics can be described by Weibull statistics. The master curve concept has been subjected to ongoing verification in solving a range of problems [e.g. 3–5]; its functionality has also been confirmed under conditions of dynamic loading [6].

To determine the reference temperature and position of the fracture toughness transition curve on the temperature axis, it is essential to carry out a minimum number of standard fracture toughness tests. These tests are relatively demanding; they involve a high consumption of experimental material. It is often difficult to use these tests for the purposes of estimating embrittlement during exploitation due to a lack of material [7]. The master curve concept brings one important advantage however. To quantify the trans-

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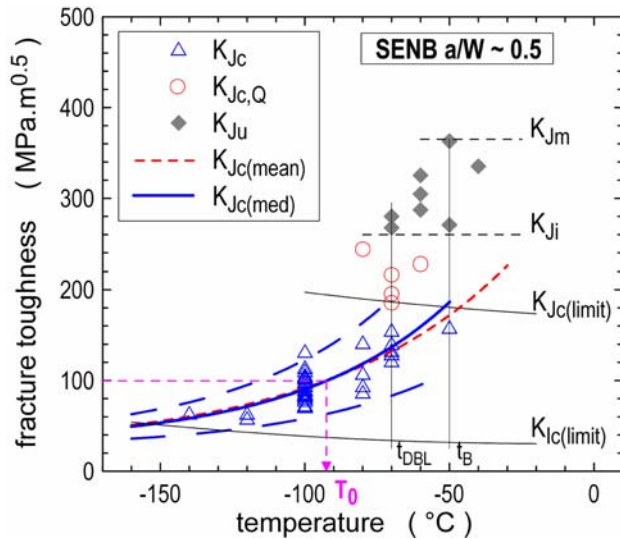


Fig. 1. Fracture toughness temperature dependence with reference temperature determination T_0 .

ition region of fracture toughness values, i.e. to determine the master curve and the scatter band, only one value, the reference temperature, is necessary to know. This may be determined either experimentally based on standard fracture toughness tests [6] and/or test by applying subsized test specimens [8, 9]. Some attempts have been also made to predict this temperature based on theoretical considerations [5, 10].

A typical example of a temperature diagram for fracture toughness of cast ferritic steel [11] is shown in Fig. 1. There are typical areas of valid fracture toughness characteristics [12]. Almost all values are lying between the lines representing the K_{Ic} validity limit and K_{Jc} validity limit in the investigated temperature interval. The full curve represents the exponential function of the master curve described by the equation [2]:

$$K_{Jc(\text{med})} = 30 + 70 \exp[0.019(T - T_0)]. \quad (1)$$

The temperature corresponding to median value equal to $100 \text{ MPa m}^{1/2}$ of fracture toughness data set in transition region is taken as reference temperature T_0 , for the particular steel the temperature $T_0 = -93^\circ\text{C}$. The dashed lines correspond to 90 % probability scatter band, described by similar equation as the previous median curve, i.e.

$$K_{Jc(0.05)} = 25.4 + 37.8 \exp[0.019(T - T_0)], \quad (2)$$

$$K_{Jc(0.95)} = 34.6 + 102.2 \exp[0.019(T - T_0)]. \quad (3)$$

The equations (2) and (3) quantify the limits for 5 and 95 % fracture probability, respectively.

Despite major progress in the quantification of

brittle fracture initiation under various loading conditions, one specific problem has not been addressed fully: the reliable determination of fracture toughness reference temperature when using other specimens than standard pre-cracked ones. One possible solution how to determine the fracture parameters is seen in the use of simpler tests, e.g. tensile tests or other tests of the local properties. It cannot be expected that a direct physical correlation will be found between diametrically different tests, e.g. fracture toughness tests on the one hand and instrumented indentation tests [13], or other small volume test techniques as small punch tests on the other hand [14, 15]. Thanks to master curve concept the existence of a single value representing the toughness transition behaviour – the reference temperature – nevertheless represents an excellent opportunity to find ways of predicting it.

Artificial neural networks (ANN) have proved to be powerful in solving complex problems of materials science [16, 17]. It is appropriate to attempt neural network analysis when problem is so complicated that a rigorous treatment is impossible or supplying uncertain unambiguous results and yet a quantitative treatment is needed [4], e.g. for transition behaviour prediction. A few studies in this area have shown that ANN analyses enable a model to be found which went the prediction of e.g. impact energy with a relatively high degree of accuracy [18, 19]. Very often processing parameters have been correlated to final properties using artificial neural networks [19]. Reliable prediction has been obtained for fatigue crack growth rate from tensile properties [20]. A few attempts have been also carried out relating the processing variables with fracture characteristics [20, 21] and/or other selected mechanical properties [22–25].

The aim of the study was to determine the usability of neural analysis for the prediction of the transition behaviour of ferritic steels, as well as to highlight the problems connected with this method. The paper presents the first findings in this area; though the research is still under way, the findings presented here are quite original and promising.

2. Materials and experimental methods

The applied materials have been of various origins. The steels selection involved the strict application of the following criteria: (i) the steels are used primarily in power engineering, (ii) the origin of the material is well guaranteed where possible by a certificate of history or manufacturing and a known geometry of the semi-finished product from which the specimens are made, and (iii) the properties of the steel cover the range of the most common microstructures and yield strengths. For the purposes of the paper a total of 29 steels and states of steel of the following types

Table 1. Steels included into investigation (the steels designated by dot included into final predictive model)

Indication	Metallurgical formula	Description	Microstructure	
	A	Fe	arema	ferrite
•	N	FeMn	sheet material as received	ferrite-pearlite
•	O	FeMn	sheet material as received	ferrite-pearlite
	P	FeMn	sheet material as received	ferrite-pearlite
•	S	FeMn	cast steel for container	ferrite
•	C	FeMn	cast steel for container	ferrite
•	E	FeMn	cast steel for container	ferrite
•	S	CrV	cold end of rotor Steti	pearlite-ferrite
•	L	42CrMo4	thick walled forging axial part	pearlite-ferrite
•	R	45Mn	R7T – railway wheelset	pearlite
•	H	CrMoV	pipes from P91	temp. mart.-bainite
•	t	NiWV	hot end from rotor Steti	temp. bainite
•	a		steel TRIP – as received	temp. bainite
•	d	CrMoV	cold end of rotor Porici	temp. bainite
	c	CrMoV	hot end for rotor Porici	temp. bainite
•	G	CrMoV	carbide triggered cleavage	temp. bainite
	F	CrMoV	dislocation triggered cleavage	temp. bainite
•	J	10Ch2MFA	RPV steel VVER 440	temp. bainite-martensite
•	T	CrNi	boiler steel	temp. bainite
•	I	CrNi	boiler steel aged	temp. bainite
•	X	15Ch2NMFAA	RPV steel VVER 1000	temp. bainite-martensite
•	Y	15Ch2NMFAA	RPV steel VVER 1000 – model	temp. bainite-martensite
	Z	15Ch2NMFAA	RPV steel VVER 1000 – model	temp. bainite-martensite
•	V	20CrNiMoV	rotor steel 500 MW – axial part	temp. bainite-martensite
•	M	20CrNiMoV	rotor steel 500 MW – surface	temp. bainite-martensite
•	B	Lo8CrNiMo	cast bainitic steel	bainite
•	K	42CrMo4	thick walled forging – surface	bainite
•	P	Lo17CrNiMo	cast bainitic steel	bainite
•	D	CrMoV	rotor steel	bainite-martensite

(see Table 1) were collected and generated:

- Arema steel and ferritic cast steels (labelled as A, S, C, E);
- low-carbon low-alloy CrMoV steels commonly used e.g. for rotors of steam power generators, in microstructural experimental state and in states following operational exposure (c, d, F, G);
- low-alloy (Cr)NiMo(V) steels in their original state and following operational exposure (s, t, M, V, D);
- advanced steels under development for thick-walled forgings (K, L);
- ferritic weldable sheet steels (N, O, p);
- nuclear reactor pressure vessel steels in basic state and model states (J, X, Y, Z);
- boiler and pipe steels with increased yield strength (T, I, H, a);
- pearlitic and bainitic steels applied in railway components (P, B, R) to cover the high yield strength end of the steels scale.

After rejecting 5 steels due to extremely low critical brittleness temperatures or data inconsistency even after repeated tests, a total of 24 data sets remained (in Table 1 designated by dot). The rejected data sets have been subjected to further detailed

analyses and are to be included into analyses later.

To determine *fracture toughness*, standard test specimens were used, with dimensions $25 \times 50 \times 240$ mm³ and demonstrably from a single semi-finished product. The specimens were positioned so that the crack propagation plane corresponded with real service conditions. In justifiable cases, especially due to the limited size of the semi-finished product, compact tension specimens were also used. The testing and evaluation of fracture toughness were carried out in accordance with the standards [26, 27].

To determine the reference temperature T_0 it was necessary to obtain at least 7 valid fracture toughness values K_{Ic} or K_{Jc} . In most cases the reference temperature was calculated applying the multi-temperature method according to the following equation:

$$\sum_{i=1}^N \frac{\exp\{c[T_i - T_0]\}}{a - K_{\min} + b \exp\{c[T_i - T_0]\}} - \sum_{i=1}^N \frac{(K_{Jc(1T)_i} - K_{\min})^4 \exp\{c[T_i - T_0]\}}{(a - K_{\min} + b \exp\{c[T_i - T_0]\})^5} = 0. \quad (4)$$

In justifiable cases the reference temperature T_0 was determined by the single-temperature method,

defined by the relation

$$T_0 = T - \frac{1}{0.019} \ln \left[\frac{K_{Jc(\text{med})} - 30}{70} \right] \quad (\text{K}). \quad (5)$$

Details of both methods are described in ASTM E 1921 standard [2]. The validity of the values thus gained was verified graphically by comparison of the generated 90 % probability band and the individual measured values.

For the purposes of standard *tensile tests*, 6 mm diameter bars were used. Standard strength and deformation properties were determined. In addition, properties were determined which were expected to display a strong direct (physical) correlation with the fracture behaviour of cracked specimens and the predicted reference temperature. These properties were true stress σ_m , σ_u and true strain values ε_{pn} , ε_u at the beginning of plastic instability and at fracture.

Tensile test specimens with circumferential notches were also included into analysis. The geometry of the test specimen was developed to ensure that even in the most ductile materials, embrittlement occurred at temperatures higher than the temperature of liquid nitrogen (V-notch angle 45°, root radius of 0.25 mm). Apart from steels T and I, in which the critical brittleness temperature was extrapolated, this behaviour was in fact observed. The objective of the tests was to determine the general yield temperature T_{gy} for the given test specimen geometry and quasistatic loading conditions. The general yield temperature was experimentally determined as temperature at which fracture occurs at the moment of the first macroplastic deformations below the notch, i.e. temperature at which the fracture stress coincides with general yield stress acting in the test specimen cross-section below the notch root. Additionally, the nominal fracture stress R_u was determined from a load at fracture F_u , in addition, total relative elongation A^* and total reduction of area at the narrowest location (neck) Z^* were obtained for general yield temperature (purely brittle fracture) and room temperature (purely ductile fracture).

The validity and compatibility of all determined data were verified on the basis of the temperature dependences and known physical (materials) relationships.

The ANN applied contained 3 layers (Fig. 2). The input layer neurons play a formal role and do not carry out any calculations – it is via these neurons that the network receives external information – input activities x_1 , x_2 , x_3 , x_4 etc. represented by selected sets of input tensile test parameters. In total, 24 numerical inputs have been tested in different combinations and one qualitative parameter (microstructure). The second layer contains hidden neurons, which are connected to the input neurons in various ways. The upper layer contains the output neuron, whose activity

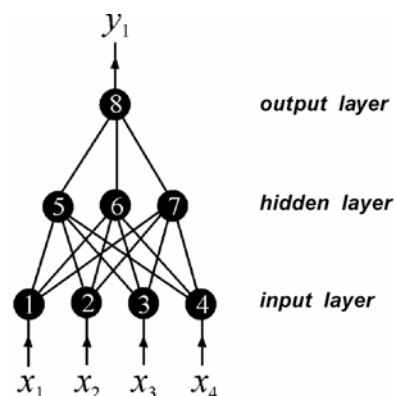


Fig. 2. Typical architecture of three-layer neural network

y_1 represents the output quantity – after preliminary tests the reference temperature T_0 of the fracture toughness temperature dependence was applied. The output neuron is connected to the hidden neurons in various ways. Each connection i - j is evaluated with a weight coefficient w_{ij} . Analogously, each hidden or output neuron i is evaluated with a threshold ϑ_i . Regularization ANN has been tested at this stage of works because of limited number of data sets and its deterministic rather than statistic character. Practical experience has shown that ANN supplied results that were far more stable and robust than those produced for complicated data sets by standard regressive models.

3. Results analysis

The above experiments produced data sets comprising over 1100 values. Partial data analyses were carried out during the course of measurement, mainly on the basis of temperature dependences of the evaluated characteristics and the comparisons of steel performance with analogous microstructure. As mentioned, these analyses led to repeated measurement or the (temporary) rejection of 5 steels from subsequent analyses as already mentioned.

One of the key tests was the determination of reference temperature T_0 . (For selected steel a correlation of measured data and curves obtained by means of master curve methodology is shown in Fig. 1). In addition to the evaluation of fracture toughness temperature diagram, Fig. 3 shows the dependence of fracture toughness on normalized temperature for the investigated steels. The figure supplies evidence for the validity of determining the reference temperature and the validity of the master curve concept for most steels. Analyses proved that the determined reference temperature can be considered entirely reliable; practically all fracture toughness values lie within the (90 %

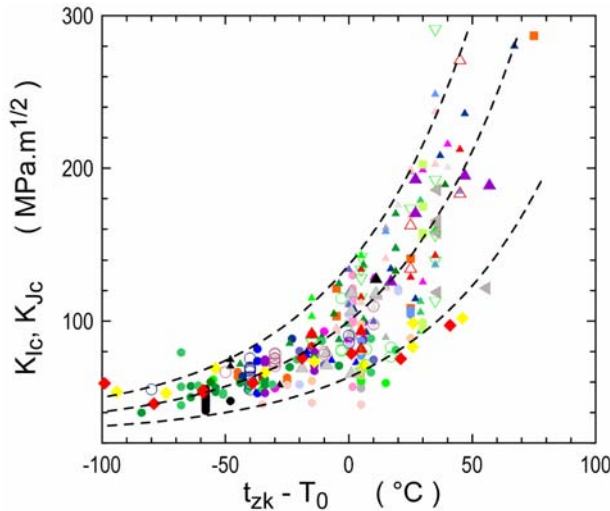


Fig. 3. Temperature dependence of fracture toughness for all investigated steels in 90 % probability scatter band of master curve.

probability) scatter band. Only steels Y and Z showed anomalous distribution of values in the band; however, in these steels coarse-grained structure was simulated and the fracture was intercrystalline, i.e., in such cases the full validity of the master curve was not expected.

It was one of the main intentions to include the tensile specimens with circumferential notches into the analyses in order to test the behaviour of the neural network in relation to failure mechanism transition. Only with bars of the selected geometry was it possible at a single quasistatic loading rate to reach two limit mechanisms – transcrystalline cleavage and ductile tearing. At the reference temperature to be get on the output side of the neural analysis there is a predominant occurrence of transcrystalline cleavage fracture, in some cases with small areas of ductile fracture and ductile fracture pre-cracking preceding to cleavage. One of the expected properties of artificial neural network should be its ability to predict the parameter corresponding to the transition area from limit parameters corresponding with lower and upper threshold values. For this purpose, the selected property of pure cleavage fracture was the general yield temperature T_{gy} determined as the temperature of coincidence of fracture force and force at the limit of macroplastic deformations. The fracture data determined at this temperature were then used as input parameters for neural analysis.

In testing the accuracy of determination of this temperature, it was interesting to compare this general yield temperature (for tensile test bars with circumferential notches) with the reference temperature (determined on the basis of fracture toughness measurement); this is summarized in Fig. 4.

The solid line shows the linear dependence gained

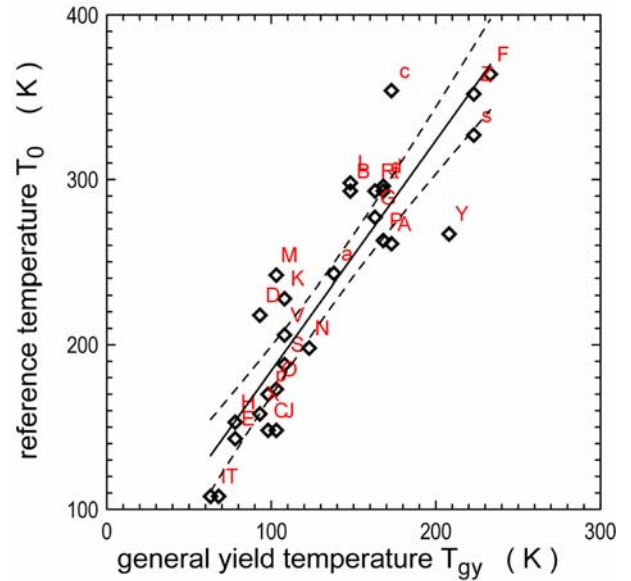


Fig. 4. Correlation of reference temperature and general yield temperature of tensile test specimen with circumferential notch.

by regression analysis (with the correlation coefficient 0.85). The correlation of both values is quite evident, but it was not ambition of authors to analyse this more deeply in this study. Only in cases where the artificial neural network showed a remarkable deviation between the predicted and experimentally determined reference temperatures was this correlation used to discover whether the deviation was caused by some error in experimental determination of data.

Because of limited number of data sets and high number of parameters on the input side the analysis was carried out in several stages: (i) The selection of suitable input attributes (i.e. those parameters on whose basis the reference temperature was to be predicted). Stochastic optimization methods were applied for this purpose. (ii) The selection of steels for the training set and for verification of the ANN mostly based on analysis of preliminary results (empirical approach). (iii) The final processing of the training set by regularization neural network and the final reference temperature prediction test.

The analyses showed reliably which input parameters unambiguously influence the prediction of reference temperature. On the input side, 25 different properties of the above-mentioned mechanical tests were investigated; in addition attributes of microstructure, hardness and instrumented indentation tests were included to these. Some of the parameters were duplicated on the input side (e.g. true fracture stress corrected and uncorrected for triaxiality). Nevertheless, the notched bar tensile test and the general yield temperature proved to be exceptionally significant. The best prediction was achieved by simultaneously using the

tensile strength at room temperature, yield strength and true fracture strain at critical brittleness temperature. A surprising result was that in smooth bars, local material properties such as true fracture strain or slope of line beyond the plastic instability limit do not belong among the descriptors with a significant influence on prediction.

The steels providing the worst prediction of reference temperature were identified in two stages. In total, 5 steels (F, Z, c, and in addition p, A) were progressively rejected from the analyses. This step improved prediction accuracy by 10 %. The probably justifiable reason for their rejection was the deviation in the fracture behaviour of the above-mentioned steels in the analysed set. This hypothesis is based on the fact that the analysed set of steels is relatively small, and so the neural network used is relatively simple. It is a justifiable assumption that increasing the quantity of input data (i.e. sets of mechanical parameters of steels included in the investigation) and using a more complex ANN will improve the network's ability to generalize, and that it will be possible to predict the reference temperature for the currently problematic steels with greater accuracy. Following the rejection of the 3 steels, the significance of the descriptors in the prediction also changed, however, the analysis confirmed the exceptional significance of the tensile test with circumferential notched bars and general yield temperature for these specimens. Among the 100 best predictions (generated for different combinations of input parameters), not one failed to include at least one of the following descriptors: general yield temperature T_0 , nominal fracture stress R_{m} , or reduction in area of notched bars Z^* .

A limiting factor in the data processing was the limited number of data sets in the training set. This problem was addressed by selecting a prediction model that was suitable for small training sets – regularization neural networks. Additionally, the data sets were not divided into the usual training and testing sets as commonly (see Chapter 2); this problem was solved by using an iterative division method, i.e. each training set progressively became a testing set.

Figure 5 shows the results of prediction using neural networks, progressively optimized both by modification of the input data set and by the selection of attributes. The deviation of predicted and measured reference temperatures lies within a relatively narrow interval. In individual cases this deviation approaches an error in the determination of reference temperature. On the basis of the above-described analyses and results, it can be claimed that the prediction of fracture toughness on the basis of reference temperature predicted from other mechanical tests is essentially possible.

In view of the highly positive results of the prediction of reference temperature, it is recommended to

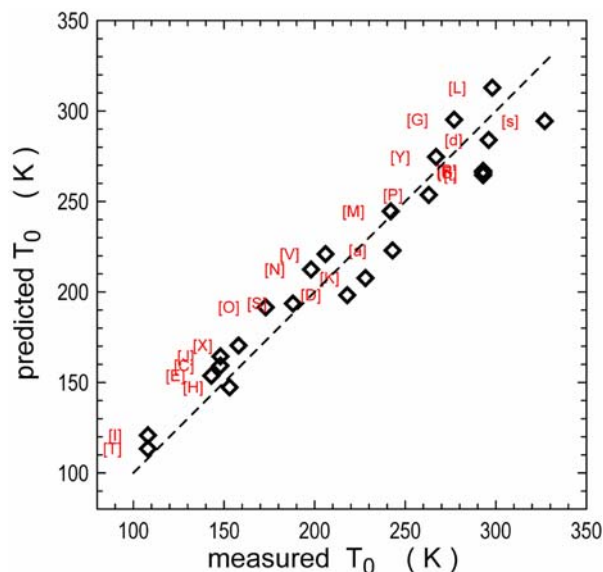


Fig. 5. Comparison of reference temperature predicted by optimized (for available data) neural network and determined by experimental measurements.

double the set of parameters, which would certainly lead to an improvement in the accuracy of reference temperature prediction and a reduction in the number of input parameters. It would also enable the neural network-based prediction model to be tested using learning based on back propagation of error; one of the advantages of this method is its better capability of generalization and prediction of output values and its lower sensitivity to the set of input parameters used.

6. Conclusion

Artificial neural network (ANN) has been applied to investigate a predictability of fracture toughness transition temperature diagram based on data from tensile tests of smooth and notched tensile test specimens. In total 24 data sets of low alloyed steels with predominantly ferritic microstructure have been applied for investigation, each consisting of 24 numerical inputs (strength and strain parameters of tensile tests), one qualitative (microstructure), and corresponding data to fracture toughness temperature diagrams. Quite promising correlation has been found between predicted and experimentally measured values of reference temperature T_0 (Fig. 4) showing the correctness of the concept.

As a limiting factor in the processing procedures the small number of data sets in the training set was found. This problem was addressed by selecting a prediction model suitable for small training sets – regularization networks. Additionally, the data sets were

not divided into the usual training and testing sets; this problem was solved by using an iterative division method, i.e. each training set progressively became a testing set.

Reference temperature T_0 localizing the fracture toughness on the temperature axis has been found as optimal parameter in the ANN output. It enables to determine fracture toughness transition curve including the scatter band for prescribed fracture probability. On the other side only one output parameter of ANN prediction enhanced an accuracy of the prediction method.

Outgoing from combinations of 24 different tensile parameters on the input side of ANN the tested alternatives revealed that key effect in prediction played the ultimate tensile strength, R_m , and true stress, σ_{pn} , at the beginning of plastic instability for smooth tensile test specimen, and, in addition, the fracture load, F_u , and nominal fracture stress, R_u , determined at general yield temperature, T_{gy} , from notched tensile specimens. The parameters that appeared to have direct physical interrelation to crack tip fracture phenomena, the slope of the true stress-true strain curve after beginning of plastic instability, the true stress σ_u and true strain value ε_u at fracture, i.e. parameters corresponding to localized deformation during necking of smooth tensile bars, have not been found as important parameters in prediction.

Good correlation between general yield temperature of tensile test bars with circumferential notches and the reference temperature determined on the basis of fracture toughness measurement has been found.

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