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PREDICTION OF FRACTURE TOUGHNESS TEMPERATURE DEPENDENCE APPLYING NEURAL NETWORK

OCENA ZAVISNOSTI ŽILAVOSTI LOMA OD TEMPERATURE PRIMENOM NEURONSKE MREŽE

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Keywords
- brittle to ductile transition
- fracture toughness
- artificial neural network
- steels

Abstract

Reference temperature localizing the fracture toughness temperature diagram on temperature axis is predicted based on tensile test data. The regularisation neural network is developed to solve the correlation of these properties. Three-point bend specimens are applied to determine fracture toughness. The fracture toughness transition dependence is quantified by means of the master curve concept enabling to represent it by using one parameter, i.e. the reference temperature. Tensile samples with circumferential notch are also examined. In total 29 data sets from low-alloy steels are applied for the analysis. A good correlation of the predicted and experimentally determined values of the reference temperature is found.

Ključne reči
- prelaz od krtog u plastično
- žilavost loma
- veštačke neuronska mreža
- čelici

Izvod

Lokalizacija temperaturskog dijagrama žilavosti loma referentnom temperaturom na temperaturnoj osi je određena na osnovu podataka ispitivanja zatezanjem. Razvijena je regularizacija neuronske mreže radi rešavanja korelacije ovih osobina. Primenjene su epruvete za savijanje u tri tačke za određivanje žilavosti loma. Krto-duktilni prelaz žilavosti loma je utvrđen primenom koncepta master krive, što je omogućilo prikaz upotrebom samo jednog parametra, na pr. referentne temperature. Uzorci za zatezanje sa obimskim zarezom su takođe proučeni. Ukupno je za analizu upotrebljeno 29 skupova podataka ispitivanja nisko legiranih čelika. Pokazuje se dobro slaganje procenjenih i eksperimentalno određenih podataka referentne temperature.

INTRODUCTION

The concept of the master curve 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. in the operational degradation of steels in power generation. The master curve concept draws purely on an engineering basis /1/. It is based on the finding that most ferritic steels with yield strength up to 750 MPa are characterised by the same shape of the fracture toughness transition curve, including the scatter band. The transition behaviour characterising 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 of the transition region /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 the 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. It is often difficult to use these tests for the purposes of estimating embrittlement during exploitation due to a lack of material /7/. The concept brings one important advantage however. To quantify the fracture toughness transition, 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 specimens /8, 9/ or 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 showing the K_{Ic} validity limit and K_{Jc} validity limit.

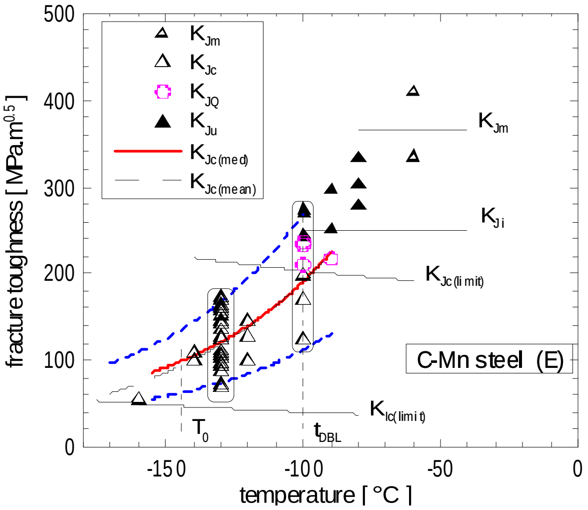

Figure 1. Fracture toughness temperature dependence with reference temperature determination T_0.
Slika 1. Zavisnost žilavosti loma sa temperaturom i određivanje referentne temperature T_0.

The non-dashed full (red) curve represents the exponential function of the master curve described by the equation, /2/,

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

The temperature corresponding to median value equal to 100 MPa·m$^{1/2}$ of fracture toughness data set in transition region is taken as reference temperature T_0; for the particular steel E, the temperature $T_0 = -147$°C. The dashed lines correspond to 90% probability scatter band, described by a similar equation as the previous median curve, i.e.

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

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

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 specimens other than standard precracked ones.

Artificial neural networks (ANN) have proved to be powerful and attractive in solving complex problems of materials science /13, 14/. It is appropriate to attempt neural network analysis when a 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 neural analyses enables a model to be found which has undergone the prediction of e.g. impact energy with a relatively high degree of accuracy /15, 16/. Quite reliable prediction is obtained for fatigue crack growth rate from tensile properties, /17/. A few attempts have been also carried out relating the processing variables with fracture characteristics /17, 18/ and/or selected mechanical properties /19-22/. A single characteristic, i.e. reference temperature, carrying the needed information on fracture behaviour and capable to quantify all the fracture toughness temperature dependence brings the opportunity to predict this quantity by ANN selection and *training* a satisfactory number of input data sets.

The aim is to determine the usability of neural analysis for the prediction of 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; and though the research is still underway, the findings presented here are quite original and promising.

ARTIFICIAL NEURAL NETWORKS

During *adaptation process (learning)*, the artificial neural networks are capable of extracting from complete data sets the correlations between the structure of training objects and their properties /23, 24/. It has even been theoretically proved that there is an universal approximator, i.e. any non-conflicting training set is ANN containing at least 2 layers of hidden neurons learnable with the required accuracy. For the application discussed here, the ANN contains 3 layers (Fig. 2). The input layer consists of input neurons, which 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. 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 y_1 represents the output of the network. 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.

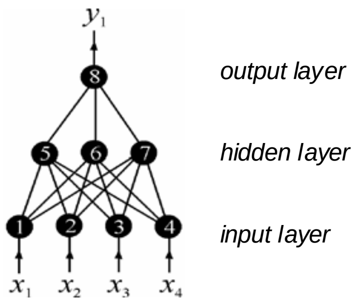

Figure 2. Typical architecture of three-layer neural network.
Slika 2. Tipična arhitektura troslojne neuronske mreže.

In the following stage, during the active process, the ANN also classifies objects that are not included in the training set, and the results gained – i.e. the response of the ANN – are compared with experimental data. This stage verifies the network's ability to generalise the data contained in the training set. Practical experience has shown that ANN give results that are more stable than those produced for complicated data sets by standard regressive models of mathematical-statistical analysis. The effectiveness of the ANN application depends heavily on the creation of the training data set which forms the basis of the adaptation process (Fig. 3), /25/. This set must contain objects, their descriptors and the required classification selected from experiments. Most commonly used for this purpose are mathematical-statistical methods of data pre-processing or artificial intelligence techniques such as clustering methods using fuzzy logic. The centres of clusters are formed by the objects of the training set; all other objects form the testing set. It is assumed that ANN adapted using objects from the training set is capable of such a level of generalization that it can also adequately interpret objects from the testing set. This ensures that the training set contains typical representatives (centres) of each cluster.

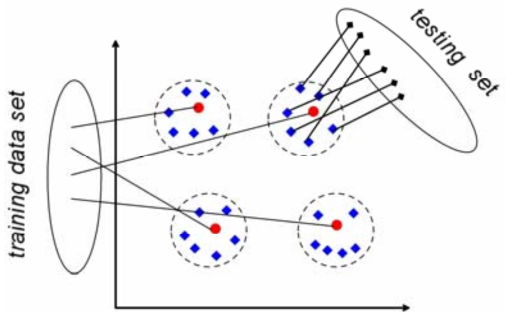

Figure 3. Separation of data sets into two disjoint sets – training/learning and testing ones.
Slika 3. Razdvajanje data skupova u dva odvojena skupa – treniranje/učenje i ispitivanje.

Objects in the training set will strongly influence the success of predictions of the output object. The training set must be formed of data sets all taken from the same material; data extracted from publications can lead to incorrect algorithms in the hidden layer of the ANN.

MATERIALS USED

The material used for testing is of various origins. For the purposes of the project a total of 29 steels and states of steel of the following types are collected:
- 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 generations, in states following operational exposure (c, d, F, G);
- low-allow (Cr)NiMo(V) steels in original state and following operational exposure (s, t, M,V, D);
- advanced steels 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 strength (T, I, H, a);
- pearlitic and bainitic steels applied in railway components (P, B, R).

TEST SPECIMENS AND METHODS

To determine fracture toughness, in most cases standard test specimens are used, with dimensions 25×50×240 mm and demonstrably from a single semi-finished product. The specimens are positioned so that the crack propagation plane corresponds with real loading conditions. In justifiable cases, especially due to the limited size of the semi-finished product, CT type specimens are also used. The testing and evaluation of fracture toughness is carried out in accordance with the standards /26, 27/.

To determine the reference temperature T_0, at least 7 valid fracture toughness values K_{Ic} or K_{Jc} are needed. In most cases the T_0 temperature is calculated applying the multi-temperature method. In justifiable cases the reference temperature T_0 is determined by single-temperature method. Details of both methods are described in ASTM E 1921 standard, /2/.

After carrying out the fracture mechanics tests, the fractured specimen halves are used to produce smaller specimens for tensile testing with smooth and notched bars.

For purposes of standard tensile tests, 6 mm diameter bars are used. Standard strength and deformation properties are determined. In addition, properties are determined that are expected to display a strong direct (physical) correlation with the fracture behaviour of cracked specimens and the predicted reference temperature. These properties are true stress σ_m, σ_u and true strain values ε_{pn}, ε_u at the beginning of plastic instability and at fracture. For these values the slope of a line characterising the tensile diagram beyond the plastic instability limit is suggested as one of the new parameters and calculated using the equation

$$\operatorname{tg}\alpha = \frac{\sigma_u - \sigma_m}{\bar{\varepsilon}_u - \bar{\varepsilon}_{pn}}. \qquad (4)$$

Tensile test specimens with circumferential notches are also included into analyses. The geometry of the test specimen is developed to ensure that even in the toughest materials, embrittlement occurred at temperatures higher than the temperature of liquid nitrogen, for details see /28/.

The objective of the tests is to determine the general yield temperature T_{gy} for the given test specimen geometry and quasistatic loading conditions. The general yield temperature is determined as temperature at which fracture occurs at the moment of the first macroplastic deformations below the notch, i.e. the 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 is determined from a load at fracture F_u and corresponding area S_u in the narrowest location of the bar:

$$R_u = \frac{F_u}{S_u} \ \text{[MPa]}. \qquad (5)$$

The total relative elongation – A^* is determined for the unstable fracture of the notched bar

$$A^* = \frac{L_u - L_0}{L_0} \cdot 100 \ [\%], \qquad (6)$$

where L_0 and L_u are specimen gauge lengths, the initial one and at fracture, in respect. Similarly, the total reduction of area at the narrowest location on the bar, Z*,

$$Z^* = \frac{S_0 - S_u}{S_0} \cdot 100 \ [\%] \qquad (7)$$

is determined for initial area and area at fracture, S_0 and S_u. All above mentioned characteristics are determined for general yield temperature (purely brittle fracture) and room temperature (purely ductile temperature).

RESULTS

The above experiments produced data sets comprising over 1100 values. Partial data analyses are 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. These analyses led to repeated measurement or the (temporary) rejection of 5 steels from subsequent analyses as already mentioned.

One of the key tests is the determination of reference temperature T_0. (For the 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. 4 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% probability) scatter band. Only steels Y and Z showed anomalous distribution of values in the band; however in these steels coarse-grained structure is simulated and the fracture is intercrystalline, i.e. in such cases the full validity of the master curve was not expected.

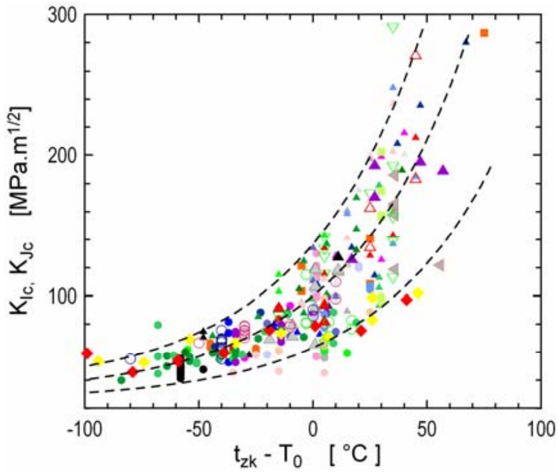

Figure 4. Fracture toughness temperature dependence for all investigated steels in 90% probability scatter band.
Slika 4. Zavisnost žilavosti loma od temperature za sve ispitivane čelike, sa verovatnoćom rasipanja 90%.

One of the main intentions was 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 in order to 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 is the critical brittleness temperature determined as the temperature of coincidence of fracture force and force at the limit of macroplastic deformations. Fracture data determined at this temperature are then used as input parameters for neural analysis.

In testing the accuracy of the determination of this temperature, it is interesting to compare this general yield temperature (for notched tensile test bars) with the reference temperature (determined on the basis of fracture toughness measurement); this is summarized in Fig. 5. The solid line shows the linear dependence gained by regression analysis (with the correlation coefficient 0.85). The correlation of both values is quite evident, but it was no ambition of authors to analyse this more deeply in this study. Only in cases where the ANN 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.

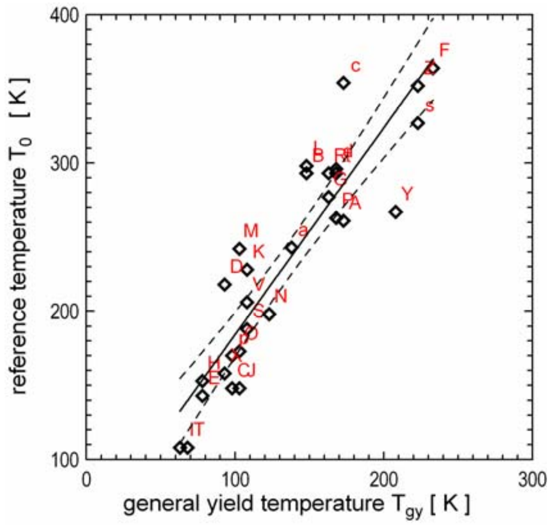

Figure 5. Correlation of reference temperature and general yield temperature of notched tensile test specimens.
Slika 5. Korelacija referentne temperature i temperature opšteg tečenja za zatezne epruvete sa zarezom.

Because of limited number of data sets and high number of parameters on the input side, the analysis is 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 optimisation methods are 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 regularisation neural network and the final reference temperature prediction test.

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 are investigated; in addition attributes of microstructure, hardness and instrumented indentation tests are included to these. Some of the parameters are 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 is achieved by simultaneously using the tensile strength at room temperature, yield strength and true fracture strain at critical brittleness temperature. A surprising result is 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 are identified in two stages. In total, 5 steels (F, Z, c and, in addition p, A) are progressively rejected from the analyses. This step improved prediction accuracy by 10%. The justifiable reason for their rejection is the deviation in the fracture behaviour of the 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 was 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_{gy}, nominal fracture stress R_u, or reduction in area of notched bars $Z*$.

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

Figure 6 shows the results of prediction using neural networks, progressively optimised 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. The priority task for further optimisation of the procedure is the expansion of the set of steels, which will make it possible to improve accuracy and reliability to the level required for industrial applications.

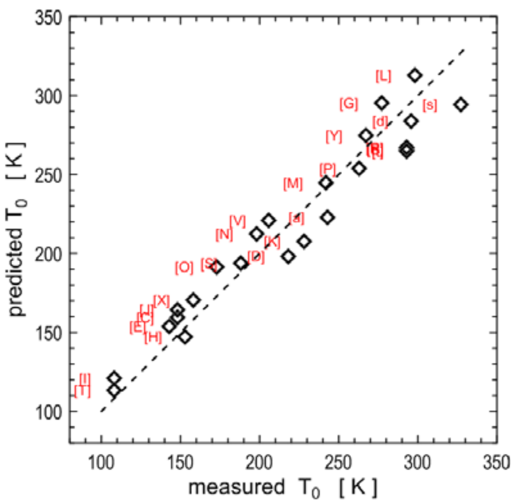

Figure 6. Comparison of reference temperature T_0 predicted by ANN and determined by experimental measurements.
Slika 6. Poređenje referentne temperature T_0 procenjene putem ANN i određene eksperimentima.

CONCLUSION

On the basis of the results achieved, it can be stated that the reference temperature characterizing fracture toughness transition behaviour in low-alloy steels with predominantly ferritic structure is predictable on the basis of selected characteristics of tensile tests.

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

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

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