MULTILAYER FEEDFORWARD NEURAL NETWORK MODELING OF THE FRACTURE MECHANICS PARAMETERS FOR THE ZR-2.5%NB PRESSURE TUBE

VASILE RADU, LIVIA STOICA, ALEXANDRA JINGA, ALEXANDRU NITU, VIOREL IONESCU, DENISA TOMA, VALENTIN OLARU
Institute for Nuclear Research (RATEN ICN) Piteşti, Romania
e-mail: vasile.radu@nuclear.ro

Abstract

CANDU reactor uses Zr-2.5Nb alloy pressure tubes as the primary coolant containment. Fracture toughness properties of the pressure tubes are required for evaluation of fracture initiation and leak-before-break. This paper presents Multilayer Feedforward Neural Network (MFNN) modelling of the fracture mechanics parameters for the CANDU pressure tube Zr-2.5%Nb alloy. The database for MFNN model used an experimental study on the effects of hydride morphology and test temperature on axial fracture toughness of a cold-worked, unirradiated Zr-2.5Nb pressure tube. The specimens were prepared from one tube section containing as-received hydrogen concentration and another section with 70 ppm hydrogen. The hydride morphologies were characterized by a parameter referred to as the hydride continuity coefficient (HCC), providing a measure of the extent to which the hydrides were reoriented concerning the applied stress direction. Partially reoriented hydrides with HCC between 0.3-0.4 were formed under the stress and temperature cycles used to precipitate the hydrides. J-R curves characterized the fracture behaviour of the specimens tested at five different temperatures: 25ºC (room temperature), 100ºC, 150ºC, 200ºC and 250ºC. The Multilayered Feedforward Neural Network model was optimised and implemented in the MATLAB environment. For two fracture mechanics parameters, namely the stress intensity factor at maximum load K_{ml}, and the J-integral at maximum load, J_{ml}, the standalone equations were obtained as a function of the following parameters: testing temperature, HHC factor, yield stress, and ultimate tensile strength. The predicted results using MFNN model were compared with the experimental ones, and a good agreement was obtained. The paper was prepared in the framework of research activities carried out in the national R&D Fuel Channel programme (coordinated by RATEN ICN), focused on the structural integrity assessments of the CANDU fuel channels.

Keywords: *Zr-2.5Nb pressure tube, fracture toughness, neural network model*

Introduction

For the Zr-2.5% Nb pressure tubes in-service evaluation, and to initiate rupture and verify the Leak-Before-Break (LBB) argument, it is necessary to know the fracture toughness properties for relatively high concentrations of hydrogen, in particular, and with various hydrides morphologies. This is especially important for tubes that have been operating in the reactor for a long time, and the equivalent hydrogen concentration increases throughout the volume of the tube. Overall, there are insufficient data on the Zr-2.5% Nb fracture toughness and its dependence on hydrogen concentration and hydride morphology, especially for high hydrogen concentrations and hydride morphology specific to the CANDU reactor conditions of operation. This required an extensive research program to obtain additional information on Zr-2.5% Nb material (cold processed, irradiated and non-irradiated) and to understand the Zr-2.5% Nb fracture properties depending on the hydrogen concentration and hydride morphology, which are representative for reactor operating conditions.

In this paper, a study is performed on the application of the method of artificial neural networks to predict the pressure tube (Zr-2.5% Nb alloy) fracture toughness, for high hydrogen concentrations and in the presence of the hydride reorientation phenomenon after hydrogen accumulation. The analysis of the paper is based on data taken from the literature, mentioned in [1]. In the mentioned paper are presented the results obtained from the fracture toughness tests on Compact-Tension (CT) samples manufactured from pressure tube segments, Zr-2.5% Nb alloy. The non-irradiated CT samples were prepared from a section of a pressure tube containing hydrogen at as-received concentration and another section from the same tube which was electrolytically hydrided at 70 ppm. The hydride reorientation was performed in the hydrided tube section in 10 thermal cycles under tensile stress applied in a circumferential direction (hoop stress) of 160 MPa. Hydride morphology was characterized by the hydride continuity coefficient (HCC) parameter. The hydrides partially reoriented with HCC = 0.3-0.4 were formed under mechanical stress and temperature cycles used for hydride precipitation. J-R fracture toughness curves were generated to characterize the fracture behaviour of the tested samples at 5 different temperatures: T_{RT} (25°C), 100°C, 150°C, 200°C, and 250°C, respectively.

The tests indicated that for as-received samples, the fracture strength is relatively high at room temperature and is not significantly affected by the temperature in the range of T_{RT} and 250°C. For samples with a hydrogen content of 70 ppm, containing partially reoriented hydrides, the material toughness is significantly lower than the one for as-received samples at T_{RT}.

Modelling the materials behaviour by the neural networks method is fundamentally different from that based on mathematical and parametric modelling of materials. In this sense, modelling through neural networks needs all the primary information on the materials behaviour, which comes from the experimental data set analysis, considering both the specific thermal-mechanical stress and the working environment conditions. One of the important features of the neural network model is that this model can describe, for example, very complex relationships between material parameters, mechanical stress and environment.

The multilayered Feedforward Neural Network (MFNN) model is applied to model the fracture toughness of the Zr-2.5% Nb alloy, represented by the parameters of fracture toughness, K_{ml} and J_{ml}.

Modelling the thermo-mechanical behaviour of structural materials with the artificial neural networks method

The modelling of the thermo-mechanical behaviour of structural materials with the method of artificial neural networks was established as an application method in the 90's [2-4]. It allows describing extremely complex relationships between the mechanical stresses applied to a structural component and the response characteristics (deformations, initiation or propagation of cracks, etc.) achieved, by using several parameters of influence.

To apply modelling with artificial neural networks, the information contained in the experimental data sets is necessary, which implicitly characterizes different aspects of the constitutive behaviour of a material. The ability to predict an artificial neural model of a certain constitutive behaviour of structural material is directly related to the volume of information contained in the experimental database [5].

The neural network method is a modern technique of great complexity in full progress [6] and it can overcome certain difficulties encountered by parametric models. Thus, the method of neural networks proved to be superior in many situations where it was necessary to extrapolate representative experimental data contained in databases with many parameters and models that can later be integrated into software programs for behaviour analysis and prediction.

The artificial neural network method can be applied in any situation where a prediction relationship between input and output variables is required.

Some features of using the artificial neural network are outlined below [7-10]. The artificial neural network can be seen as a mathematical-programmable instrument that takes a numerical input and generates a numerical output. To do this it has a transfer function of the chosen unit so that it can accept an input from a certain range of values and produces an output in a finite range of values. Even though the input may be in some range, there is a saturation effect, so the neural unit is sensitive to a practically finite input range. The most common transfer function used is the *sigmoid* function. For this situation, the output is in the range (0, 1) and the input is sensitive to a range not higher than (-1, +1). This type of function is continuous and differentiable, features that are important for the neural network to perform learning algorithms (training algorithm).

An artificial neural network that works well when is used as an approximation tool is the Multilayer Feedforward Neural Network (MFNN) or Multilayer Neuronal Network. The MFNN neural network is the most popular network architecture used today in nonlinear neural modelling. In this type of network, each unit performs a weighted amount of input data and passes this activation level through a transfer function. The units are topologically placed in layers and the information propagation takes place only from the input to the output (hence the name of the *feedforward network*).

A constructive feature is the sets of elementary neutrons grouped in so-called "layers", which provide connection similarities. As for terminology, we identify an *input* layer, an *output* layer, all other layers being called *hidden* layers. In this type of network, the specific structure causes a neuron in one layer to have connections with other neurons in other layers. Therefore, the network can be interpreted as an *input-output* model with influence and threshold parameters, which help obtaining the desired modelling.

Such artificial neural networks can model complex functions with several layers and several neurons in each layer, respectively, that can be optimized. Therefore, an important step in the MFNN neural network designing (choice) is to specify the number of hidden layers and the number of units in these layers.

An MFNN network such as the one shown in Fig. 1 can be used as a tool for approximating the functions of several variables. This network type will be used to evaluate the toughness of CANDU pressure tube, Zr-2.5% Nb alloy.

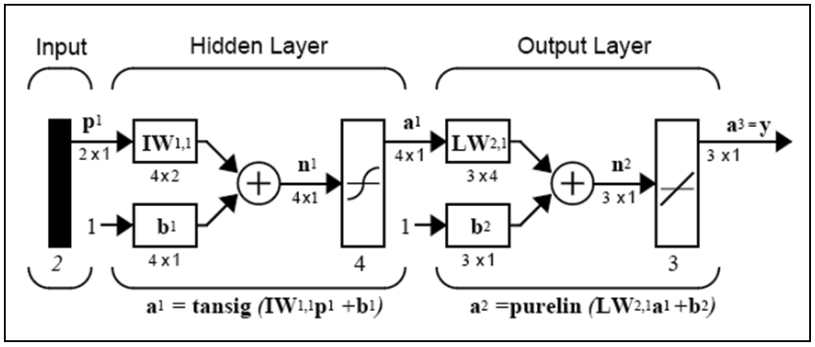


Fig.1 Two-layer MFNN network

Material properties and fracture mechanics parameters of pressure tubes, Zr-2.5% Nb alloy

The model of the fracture toughness that is the subject of this paper is based on the experimental results on the tensile strength of the Zr-2.5% Nb alloy taken from [1]. Below are some considerations of the material properties, which characterize the samples used in the tests of fracture mechanics, having the hydrides morphology at a Hydrogen concentration of 70 ppm. Previous studies have shown that the tensile strength of the Zr-2.5% Nb pressure tube material is affected by the hydrides morphology. Hydride reorientation refers to the formation of hydride morphology in the section of the pressure tube under specifically applied stress and a sequence of thermal cycles representative for the operation in the reactor.

The J-integral evaluation of the samples tested in [1] followed the procedure given in ASTM E1820 [11] for Compact-Tension (CT) samples. The determination of the various parameters of fracture mechanics depends on the behaviour of the CT sample crack increasing. There are mainly two scenarios: one refers to crack instability before unstable tearing (fragile samples) and another refers to stable tearing before unstable rupture (ductile samples). For fragile samples, a single fracture toughness parameter can be determined that characterizes fracture instability. For the samples characterized by ductile rupture, the J-R curve for each sample was calculated.

The material properties used in the J-integral evaluation include: Young's modulus (E), Poisson's ratio (υ), yield stress (σ_Y). The υ value was considered 0.4, regardless of temperature. To calculate J-integral at other temperatures (100°C, 150°C, 200°C), E and σ_Y were estimated using the empirical relations [1]. It should be noted that the tensile data on yield stress and tensile strength were obtained from tensile tests on samples with a nominal hydrogen concentration (as-received). Tensile tests were not performed on hydrated samples with reoriented hydrides.

To assess the pop-in significance, the procedure given in ASTM E1820 Section A4 was used. To analyze the test results [1], two parameters of rupture mechanics were used, namely: J_{ml} and K_{ml}. J_{ml} parameter is the J-integral at maximum load; K_{ml} parameter is the linear-elastic stress intensity factor, obtained from J_{ml} by using the relation:

$$K_{ml} = \sqrt{E \cdot J_{ml}} \tag{1}$$

MFNN model to predict the toughness of K_{ml} parameter

To model by the artificial neural networks method, using the Multilayer Feedforward Neural Network (MFNN) methodology, the fracture toughness of the Zr-2.5% Nb alloy, rendered by the K_{ml} parameter, the experimental data reported in [1] were used. The K_{ml} parameter represents the critical stress intensity factor, obtained from the J-integral curve at the point of maximum mechanical load, according to relation (1). Four parameters were used to drive the artificial neural network, namely:

- Test temperature, in degrees Celsius (°C), T;
- Yield stress, $\sigma_{0.2}$;
- Ultimate tensile strength, σ_{UTS};
- Hydride continuity factor (HCC), measuring the degree of reorientation of hydrides in the radial direction.

The equation obtained using the Matlab work environment for the MFNN model is based on the experimental results from [1] and is given below:

$$K_{ml}(T,\sigma_{0.2},\sigma_r,HCC) = \frac{28.23852153}{\exp(7.771349206 - 1.029643034\cdot S02 - 0.945794485\cdot Sr - 4.12715487\cdot T - 33.94890765\cdot HCC) + 1.0} + \frac{38.53338589}{\exp(1.323081777\cdot S02 - 41.87928933\cdot HCC + 1.593530892\cdot Sr - 5.461014499\cdot T + 18.07930676) + 1.0} - \frac{30.18762037}{\exp(22.09145988\cdot HCC + 3.014663739\cdot S02 + 3.791711272\cdot Sr - 16.08472515\cdot T + 17.70576941) + 1.0} - \frac{47.66333333}{\exp(16.95240766\cdot S02 - 876.719379\cdot HCC - 16.68948205\cdot Sr + 11.34866809\cdot T + 2.912439979) + 1.0} - \frac{40.53634935}{\exp(17.12130057\cdot HCC - 15.05698533\cdot S02 + 14.86193691\cdot Sr + 20.59289028\cdot T - 30.5320525) + 1.0} + 83.39147847 \tag{2}$$

Here S02 is yield stress, $\sigma_{0.2}$, and Sr is σ_{UTS} .

The comparative analysis, depending on the temperature, between the experimental results and those obtained by the MFNN model with equation (2) is shown in Fig. 2. At a temperature of 100°C there is a brittle-ductile transition, characteristic for samples of Zr-2.5% Nb with hydrides reoriented to a concentration of 70 ppm hydrogen, as noted by the authors of [1]. Up to this temperature, the behaviour of the samples is defined as brittle, with low values of the K_{ml} factor, after which there is a mixed behaviour of the ductile-brittle type up to a temperature of 250°C.

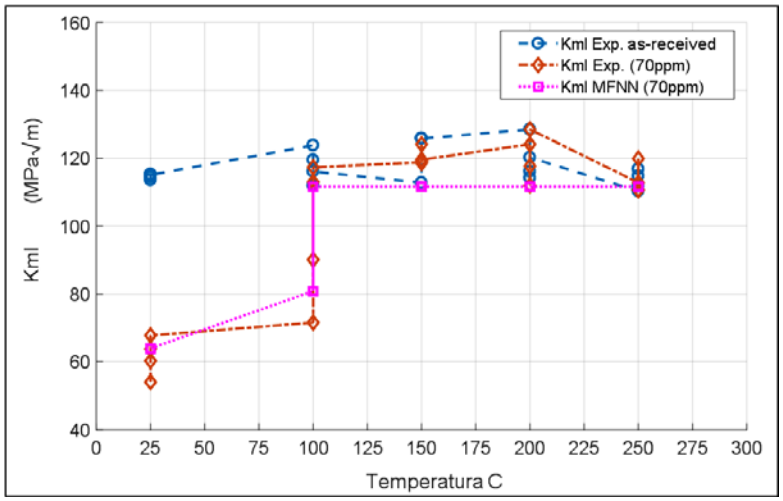


Fig. 2. Comparative analysis between experimental values and prediction for K_{ml} depending on test temperature (nominal hydrogen and 70 ppm)

It should be noted that this brittle-ductile transition, which takes place at a temperature of 100°C, is very well simulated by the neural mathematical model described by Eq. (2).

MFNN model to predict the toughness of J_{ml} parameter

The methodology of the Unidirectional Multilayer Neural Network (MFNN) was also used to model the fracture toughness of the Zr-2.5% Nb alloy, by the J_{ml} parameter. As in the previous section, the experimental data reported in [1] were used. The J_{ml} parameter is the J-integral at the maximum load applied in the fracture mechanics test. In the modelling, four parameters were used to drive the artificial neural network model, as in the previous chapter.

The equation obtained using the Matlab work environment for the MFNN model of the J_{ml} parameter, through the work routines is the following:

$$J_{ml}\left(T,\sigma_{0.2},\sigma_r,HCC\right) = \frac{45.63569355}{exp(25.44054428 - 0.5694073303\cdot S02 - 0.6488315982\cdot Sr - 0.06683049923\cdot T - 18.74709736\cdot HCC) + 1.0} - \frac{11.63211653}{exp(0.3989864095\cdot Sr - 0.8948034149\cdot S02 - 1.281945411\cdot HCC + 1.254630779\cdot T + 20.40806795) + 1.0} + \frac{86.25104354}{exp(92.55553704\cdot HCC - 0.2602931492\cdot S02 + 0.323678966\cdot Sr - 0.9385679409\cdot T - 6.768015808) + 1.0} - \frac{46.0163242}{exp(28.90470081\cdot HCC + 1.560987233\cdot S02 + 1.652560795\cdot Sr + 2.306560897\cdot T - 5.330530763) + 1.0} + \frac{47.71094916}{exp(43.19739127\cdot HCC - 0.1025110845\cdot S02 - 0.1100210945\cdot Sr - 1.430767008\cdot T + 3.036666645) + 1.0} - 37.65437293 \quad (3)$$

By comparative analysis between the experimental results and those obtained by the MFNN model given by Eq. (3), as a function of temperature, a good agreement can be observed in the MFNN model prediction shown in Fig. 3. Even in this case, brittle-ductile transition characteristic of the Zr-2.5% Nb samples with reoriented hydrides (HCC = 0.3-0.4), at a concentration of 70 ppm hydrogen, can be noticed at a temperature of 100°C.

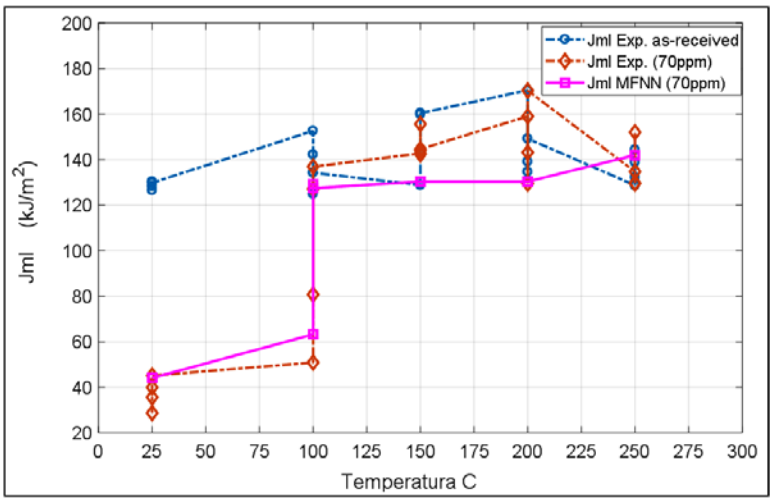


Fig.3. Comparative analysis between experimental values and prediction for J_{ml} depending on test temperature (nominal hydrogen and 70 ppm)

Up to this temperature, the behaviour is defined as brittle, with low values of the J_{ml} factor, after which there is a mixed behaviour, ductile-brittle type, up to a temperature of 250°C.

It should be noted that this brittle-ductile transition, which takes place at a temperature of 100°C, is very well simulated by the neural mathematical model described by Eq. (3).

Conclusions

CANDU reactor uses Zr-2.5%Nb alloy pressure tubes as the primary containment. Fracture toughness properties of the pressure tubes are required for evaluation of fracture initiation and leak-before-break.

This paper aims to present the Multilayer Feedforward Neural Network (MFNN) modelling of the fracture mechanics parameters for CANDU pressure tube Zr-2.5%Nb alloy. The MFNN model was optimised and implemented in the MATLAB programming environment. This led to creation of two applications to obtain the rupture mechanics parameters K_{ml} (stress intensity factor at maximum load) and J_{ml} (J-integral at maximum load), which are considered defining for the fracture toughness of the CANDU pressure tube, Zr-2.5% Nb alloy.

In order to study the influence of hydrogen concentration, hydride reorientation and temperature on the fracture toughness, experimental data from the Canadian scientific reference literature were used.

Taken into consideration the prediction functions, the results obtained by modelling the MFNN for the two parameters K_{ml} and J_{ml}, were compared with the experimental data. A good concordance was obtained, which confirms the prediction capability of the models.

The study is part of the structural integrity assessments of the CANDU fuel channels, being carried out in the framework of research activities carried out in the Fuel Channel Research Programme.

References

[1] Cui, J., Shek, G.K. (2009) ″Effects of Hydride Morphology and Test Temperature on Fracture Toughness of Zr-2.5Nb Pressure Tube Material″, Proc. of the ASME 2009 Pressure Vessels and Piping Division Conf. PVP2009, PVP2009-77260, Prague, Czech Republic.

[2] Reda Taha, M.M., Noureldin, A., El-Sheimy, N., Shrive, N.G. (2003) ″Artificial neural networks for predicting creep with an example application to structural masonry″, *Can. J. Civ. Eng.* Vol. 30, pp. 523–532.

[3] Jung, S., Ghaboussi, J. (2006) ″Neural network constitutive model for rate-dependent materials″, *Computers and Structures*, Vol. 84, pp. 955–963.

[4] Wang, N., Tu, S.-T., Xuan, F.-Z. (2013) ″A novel prediction method of creep rupture life of 9–12% chromium ferritic steel based on abductive network″, *Engineering Failure Analysis*, Vol. 31, pp. 302–310

[5] Bhadeshia, H.K.D.H. (1999) ″Neural Networks in Materials Science″, *ISIJ International*, Vol. 39 (10), pp. 966-979

[6] Bhadeshia, H.K.D.H. (2003) ″Mechanisms and Models for Creep Deformation and Rupture″, *Comprehensive Structural Integrity*, Vol. 5, pp. 1-23, Elsevier.

[7] Haykin, S. (1999) *″Neural Networks, A comprehensive foundation″*, Prentice-Hall Int. Editions Series, Pearson Education.

[8] Hagan, M.T., Demuth, H., Beale, M. (1996) *″Neural Network Design″*, PWS Publishing Co., Boston, USA.

[9] Demuth, H., Beale, M., Hagan, M.T. (2006) *″Neural Network Toolbox 5″*, User's Guide, The MathWorks Inc. Natick, MA, USA.

[10] Beale, M.H., Hagan, M.T., Demuth, H.B. (2010) *″Neural Network Toolbox™ 7″*, User's Guide, The MathWorks Inc. Natick, MA, USA.

[11] *** (2011) *″ASTM E1820-18: Standard Test Method for Measurement of Fracture Toughness″*, ASTM Int., USA.