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Bootstrap calculation of ultimate strength temperature maxima for neutron irradiated ferritic/martensitic steels

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Abstract

The dependence of mechanical properties of ferritic/martensitic (F/M) steels on irradiation temperature is of interest because these steels are used as structural materials for fast, fusion reactors and accelerator driven systems. Experimental data demonstrating temperature peaks in physical and mechanical properties of neutron irradiated pure iron, nickel, vanadium, and austenitic stainless steels are available in the literature. A lack of such an information for F/M steels forces one to apply a computational mathematical–statistical modeling methods. The bootstrap procedure is one of such methods that allows us to obtain the necessary statistical characteristics using only a sample of limited size. In the present work this procedure is used for modeling the frequency distribution histograms of ultimate strength temperature peaks in pure iron and Russian F/M steels EP-450 and EP-823. Results of fitting the sums of Lorentz or Gauss functions to the calculated distributions are presented. It is concluded that there are two temperature (at 360 and 390 °C) peaks of the ultimate strength in EP-450 steel and single peak at 390 °C in EP-823.

1. Introduction

Experimental data demonstrating the temperature peaks of physical and mechanical properties of pure iron, nickel, vanadium, and also in Fe–Cr–Ni alloys in the 200–700 °C range of irradiation and test temperatures have been presented in Refs. [1–7]. Temperature peaks of swelling were observed in post-irradiation examinations of austenitic stainless steels. The simulation using an artificial neural network of the ultimate strength of neutron irradiated ferritic/martensitic (F/M) steels has revealed a maximum of the strength located at ≈400 °C, the nature of which is unclear yet. Since F/M steels constitute structural materials for fast and fusion reactors, an investigation of the dependence on irradiation temperature of their short-term mechanical properties is of interest from both scientific and practical points of view. Expensive reactor experiments are needed for revealing such dependencies with a confidence. Unfortunately, for the present such experiments seem to be improbable.

A lack of the experimental information forces one to resort to mathematical–statistical modeling

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using computational methods. The bootstrap procedure is one of such methods that allows us to obtain the necessary statistical characteristics using only a sample of limited size [8]. The main objective of the present work consists of an application of the bootstrap-method for simulation to obtain models for frequency distribution histograms of ultimate strength σ_u temperature peaks in pure iron and Russian F/M steels EP-450 and EP-823. In addition, the results of fitting the sums of Lorentz or Gauss functions to the calculated distributions are presented.

2. Simulation method

A multilayer feed forward network (with two hidden layers) is used to represent the dependence of short-term mechanical properties of F/M steels on irradiation temperature, dose, test temperature on the distribution of temperature peaks of the ultimate strength σ_u. Training of the artificial neural network has been carried out using an experimental test sample for specimens made of EP-852, EP-450, EP-823 steels. The sample consists of 400 rows and contains the information accumulated by different authors for 40 years of investigations (see, for example, Refs. [9–12]). In the input data set exploitation conditions, chemical compositions, heat-treatment conditions, cold work levels and thermal expansion coefficients (in total, 48 parameters) are presented. The tensile ultimate strength and total elongation are the output parameters. The number of sites in hidden layers chosen by trial-error method equals 20 and 45. The structure of the neural network model looks as 48:20:45:2. The model allows to simulate irradiation conditions for samples of F/M steels with different chemical composition. Its development and verification is described in detail in Ref. [13].

In accordance with the bootstrap methodology the algorithm of simulation tests is as follows:

1. Calculation of the residuals between experimental and calculated σ_u-values.
2. Generation of bootstrap samples of σ_u by adding pseudo-experimental noise to the calculated σ_u-values by random choice of a residual from the ordered errors with returning.
3. Evaluation of the neural network model on simulated σ_u-values by considering these values as a result of the real experiment.
4. Choice of test temperatures and irradiation doses from the ranges of 20–800 C and 5–150 dpa, respectively, with equal probabilities.
5. Calculation of the ultimate strength dependence on irradiation temperature using the model corrected and determination of σ_u maximum temperature.

Steps from 2 to 5 were repeated ~300 times.

Accumulated bootstrap values of irradiation temperatures at which the ultimate strength of pure Fe, F/M steels EP-450 and EP-823 has maxima were used then for plotting the frequency distribution histograms.

3. Results of the computer experiment

In Fig. 1 such a histogram is shown for pure Fe aged at 760 °C. As it is seen, the temperatures of peaks are located in the 330–420 °C range, the peaks at the irradiation temperatures of 365, 390 and 410 °C are especially well expressed.

In Figs. 2 and 3 similar histograms are shown for neutron irradiated EP-450 and EP-823 steels preliminary normalized at 1050 °C and aged at 720 и 760 °C, respectively.

By comparing Figs. 2 and 3 with Fig. 1 one can see that the locations of σ_u-temperature peaks at 360 и 390 °C for these steels coincide with those for pure Fe. However, there is no peak at the temperature of 410 °C in the steels. In addition, it can be noted that at the temperature of 340 °C the peak of σ_u is more distinct in EP-450 steel compared with EP-823 steel, but it is absent in Fe. Possibly, alloying of iron causes a shift of ultimate strength peaks and the difference in chemical composition of the

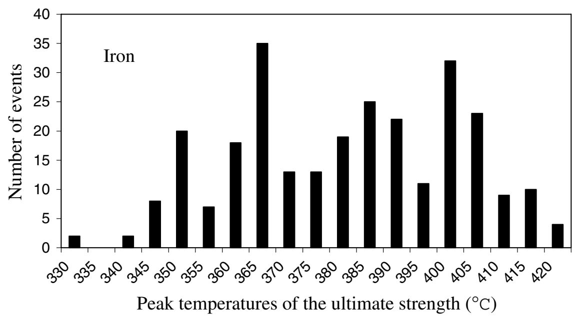

Fig. 1. The frequency distribution histogram of irradiation temperatures at which maxima of the ultimate strength of pure Fe are located.

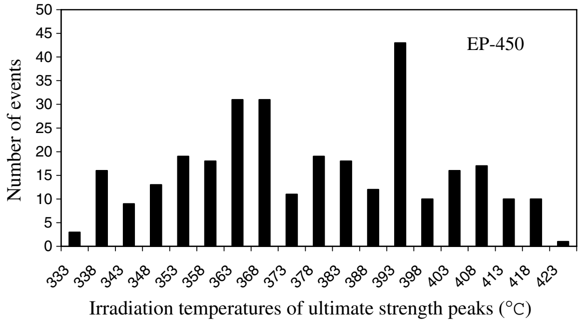

Fig. 2. The frequency distribution histogram of irradiation temperatures at which maxima of the ultimate strength of EP-450 F/M steel are located.

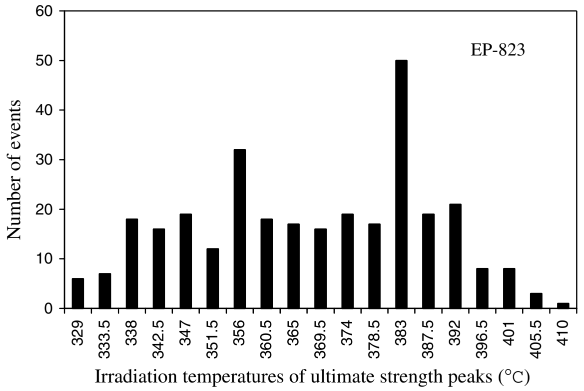

Fig. 3. The frequency distribution histogram of irradiation temperatures at which maxima of the ultimate strength of EP-823 F/M steel are located.

steels as well as their heat treatment results in a change of the temperature peak distributions.

Questions about the exact number of such maxima and the peak temperatures are important for steels being considered for application in nuclear power facilities with severe temperature conditions. These questions can be answered if to create a continuous distribution of σ_u-peak temperatures produced in the simulation experiment by using sums of Lorentz (1) or Gauss functions (2):

$$\sigma_u = A \cdot \sum_{i=1}^{k} \frac{1}{\left(t - t_i^{\max}\right)^2 + \gamma_i}, \tag{1}$$

$$\sigma_u = A \cdot \sum_{i=1}^{k} \exp\left[-\frac{\left(t - t_i^{\max}\right)^2}{\gamma_i}\right]. \tag{2}$$

In Eqs. (1) and (2) the index i denotes the peak number in the distribution; t is the peak irradiation temperature, $t_i^{\max}$ is the mean temperature of the peak, γ_i is the peak width, A is the normalization constant, and k is the total number of peaks. The identification of the sums (1) and (2) was carried out by methods of the nonlinear regression analysis. The comparison of estimates of coefficients for models (1) and (2) allows to determine the stability aspects of the estimation procedure.

The estimation of sums (1) and (2) at $k = 3$ has shown that the temperature maximum located at 340 °C is absent due to very large γ-values. Therefore, calculating the estimates of parameter was carried out under assumption that two peaks located at 360 and ≈390 °C exist. In Table 1 the results of estimating the parameters $t^{\max}$ and γ from frequency histograms for steels EP-450 and EP-823 are shown for the models (1) and (2).

As it follows from Table 1, in the model representation of the EP-450 steel histogram the temperatures of main peaks are almost identical for sums (1) and (2). The distribution histogram and curves calculated using the Eqs. (1) and (2) are shown in Fig. 4.

Table 1
Estimates of parameters for EP-450 and EP-823 steels

Model	$t_1^{\max}$, °C	$t_2^{\max}$, °C	γ_1, °C	γ_2, °C
EP-450 steel				
(1)	361	392	151	174
(2)	359	393	375	336
EP-823 steel				
(1)	354	387	148	98
(2)	364	388	1425	42

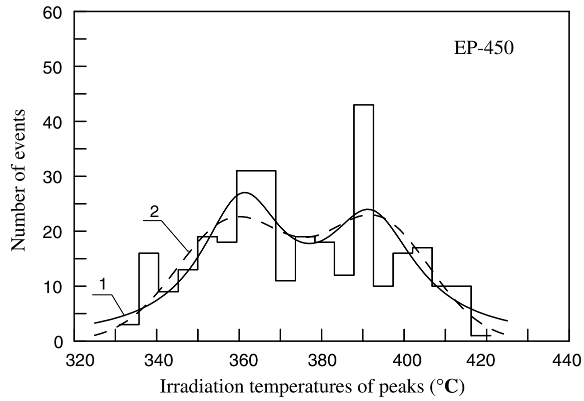

Fig. 4. Simulated distribution histogram of irradiation temperatures at which the ultimate strength of EP-450 steel has maxima and curves fitting this distribution: 1 – Eq. (1), 2 – Eq. (2) (data of Table 1).

Since the calculated curves are close each to other, one can conclude that with a high probability there are two temperature peaks of the ultimate strength in EP-450 steel. Meanwhile, shown in Table 1 lines for EP-823 steel differ, especially, in the γ_1-parameter. The value of the γ_1-parameter is so large that the peak in the vicinity of 360 °C became eroded up to equally probable values when modeling of the histogram by the sum of Gauss functions (2). From Fig. 5, which illustrates this statement, it is clearly seen that the curves calculated using the functions (1) and (2) differ. Such a difference puts under doubt the existence of the σ_u-peak at the irradiation temperature of 360 °C for EP-823 steel. Meanwhile, the calculated curves coincide in the vicinity of 390 °C, that allows to affirm that the peak of σ_u really exists at this temperature.

An independent choice of test temperature and dose (see item 4 of simulation experiment algorithm) allows to establish how each of these factors influences the peak irradiation temperatures. In Fig. 6 the data of the simulation experiment for EP-450 steel are shown in coordinates 'test temperature t_{test}-peak irradiation temperature' along with the straight line calculated using the following regression equation:

$$t = 336 + 0.09 \cdot t_{test}. \tag{3}$$

However, a uniform distribution of experimental data shown in Fig. 7 gives evidence about the absence of any relationship between doses and peak temperatures.

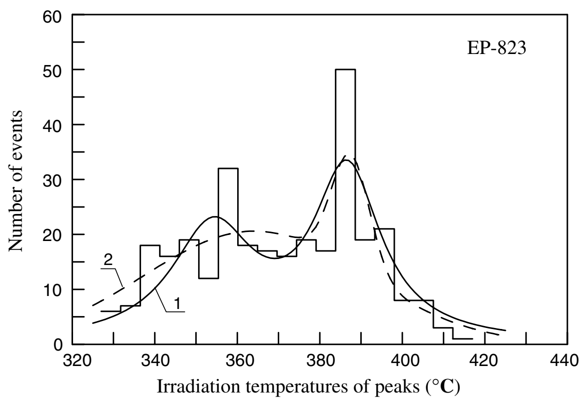

Fig. 5. Simulated distribution of irradiation temperatures at which the ultimate strength of EP-823 steel has maxima and curves fitting this distribution: 1 – Eq. (1), 2 – Eq. (2) (data of Table 1).

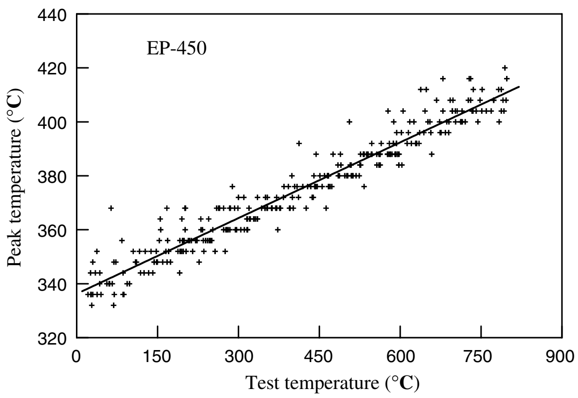

Fig. 6. Data of the simulation experiment for EP-450 steel and the straight line calculated using Eq. (3).

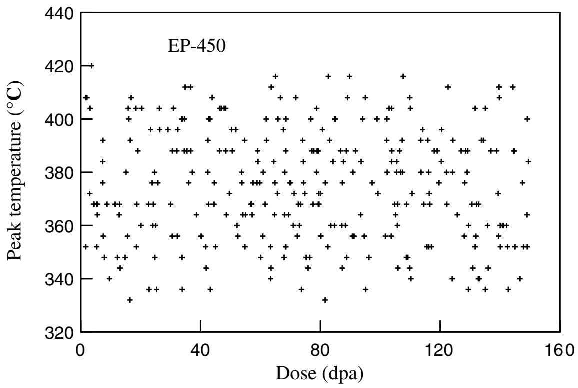

Fig. 7. Results of the simulation 'experiment'.

The similar data for pure iron and steel EP-823 demonstrate the same behavior: there is a linear relationship between peak irradiation temperatures and test temperatures, and the absence of any correlation with the dose.

4. Discussion of results

The results of the simulation experiment carried out, and also fitting the sums of bell-shaped functions to the data indicate the existence of two ultimate strength temperature peaks at ≈360 and 390 °C in EP-450 steel. For EP-823 steel one can confidently speak about the presence of the maximum σ_u at 390 °C, but the probability of maximum at 360 °C is low. From comparison of histograms of peak temperature distribution in pure iron and F/M steels it follows that alloying of iron results in a change of the peak temperature arrangement. This fact is in well agreement with data of Ref. [6]

according to which the temperature peak of the ultimate strength in pure vanadium shifts along with respect to the peaks in vanadium based alloys.

Interestingly, the maximum swelling of zone refined iron irradiated with 1.25 MeV – electrons in a high-voltage electron microscope was observed at 350 °C, but in iron implanted with oxygen and helium-at 400 °C [14]. In neutron irradiated iron and model alloys Fe–Cr the swelling peak is located at 425 °C [15]. The swelling rate of neutron irradiated EP-450 steel is maximal at temperatures around 400 °C [16]. The swelling peak temperatures for these materials are close to the ultimate strength peak temperatures revealed in bootstrap calculations for F/M steels. This fact can be considered as an indication of that the physical cause of strength and swelling temperature maxima is the same. Possibly, this cause is related to peculiarities of microstructural defects formation (voids, dislocation loops, dislocations) in iron based alloys at the specific temperatures of ≈360 °C and ≈400 °C.

An analysis of results of the present computer experiment has revealed the well expressed linear relationship between irradiation and test temperatures at which ultimate strength has maximum as well as the absence of any correlation between the dose and peak irradiation temperature. Because values of σ_u are determined by radiation defects such a behavior should correlate with the temperature behavior of, at least, one type of the defects. The results of the microstructural investigation of EP-450 steel irradiated with neutrons at in wide ranges of temperatures and doses unequivocally demonstrate that the dislocation loop concentration depends strongly on irradiation temperature and rather slightly on dose [16].

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