

# Simulation of the main components of a nuclear reactor under load, made of ultrafine-grained steel AISI-321 in the normal and irradiated state

Abdrakhman Naizabekov<sup>1</sup>, Evgeniy Panin<sup>2</sup>, Andrey Tolkushkin<sup>3</sup>, Daniyar Zhumagaliev<sup>1</sup>

<sup>1</sup>Rudny Industrial Institute, Rudny, Kazakhstan

<sup>2</sup>Karaganda Industrial University, Temirtau, Kazakhstan

<sup>3</sup>Ural Federal University, Yekaterinburg, Russia  
cooper802@mail.ru

**Abstract:** The creation and calculation of computer models of various products under load with the properties of UFG materials in the normal and irradiated state was performed. To model the UFG properties of non-irradiated AISI-321 steel, hardening curves were constructed based on the Hall-Petch equation for the base state of the material at a grain size of 1500 nm and for two UFG states (with grain sizes of 700 and 200 nm). To simulate the properties of irradiated AISI-321 steel, plastometric tests were performed using uniaxial compression of cylindrical samples at constant values of the strain rate of  $1 \text{ s}^{-1}$  and the temperature of  $20^\circ\text{C}$  on the "Gleeble 3800" plastometric unit. Fast neutron fluence with the following values was selected as a variable parameter:  $0.5 \cdot 10^{18} \text{ n/cm}^2$ ,  $1 \cdot 10^{18} \text{ n/cm}^2$ ,  $0.5 \cdot 10^{19} \text{ n/cm}^2$ ,  $1 \cdot 10^{19} \text{ n/cm}^2$ . The maximum operating pressure of 340 MPa was used as a static load. The simulation results showed that for both parts, the use of the material in the UFG state is the most appropriate solution.

**Keywords:** FEM, UFG STRUCTURE, IRRADIATION, STRESS

## 1. Introduction

The most important components of a nuclear reactor are the elements directly in contact with the nuclear fuel tablets: fuel assembly and fuel element.

The body of the fuel assembly is a metal structure (figure 1) containing fissionable substances and intended for generating thermal energy in a nuclear reactor by performing a controlled nuclear reaction. Usually it is a tetrahedral (PWR) or hexahedral (VVER) beam of fuel rods with a length of 2.5–3.5 m (which approximately corresponds to the height of the core) and a diameter of 30–40 cm, made of stainless steel or a zirconium alloy (to reduce neutron absorption) [1].



Figure 1 - Typical design of fuel assembly

The body of the fuel assembly has a total length of 3500 mm, there are three characteristic sections that differ not only in shape, but also in purpose. The head part is a body of rotation, the upper section of which has a conical shape, and the lower section has a cylindrical shape. It is designed for loading fuel elements, as well as fixing fuel assemblies in the overall design of the reactor. The wall thickness in this zone varies from 4 to 7 mm. The bottom part is also a cylindrical body of rotation. It is designed for loading fuel elements, as well as fixing fuel assemblies in the overall reactor structure by means of a threaded connection. The wall thickness in this zone is 4 mm. The longest central part with a length of more than 2500 mm has a hexagonal cross-section with a "turnkey" size of 96 mm and is intended for direct maintenance of fuel elements in the amount of 37 pieces. The wall thickness in this zone is 4 mm.

The geometry of the fuel element is a cylindrical body with a cavity into which uranium oxide tablets are loaded [1]. There are also three zones – head, central and bottom. But, unlike the hull, all these zones have a cylindrical shape. Wall thickness in all zones of the fuel elements is 0.45 mm.

## 2. Creation of models of UFG-materials

To create a model of AISI-321 steel in an ultrafine-grained state, it is necessary to put the values of mechanical characteristics corresponding to this state in the material database. The key parameter for this is the yield strength of the material, i.e. the mechanical characteristic of the material that characterizes the stress at which the deformations continue to grow without increasing the load. At room temperature, the yield strength is 270 MPa [2].

However, this value characterizes AISI-321 steel in the pre-deformation state, without any level of hardening. To determine the yield strength values for different grain size values, it is recommended to use the Hall-Petch ratio [3-4], which is the following relationship:

$$\sigma_Y = \sigma_0 + k d^{-1/2}, \quad (1)$$

where  $\sigma_Y$  – desired yield strength value, MPa;

$\sigma_0$  – stress impeding the dislocations movement, MPa;

$k$  – constant, depending on the properties of a particular material;

$d$  – grain size, microns.

In the course of experimental studies, a grain size range of 200–700 nm was obtained. Taking into account that when modeling properties, it is necessary to assume a uniform initial distribution of properties, we will set the limits of this range as the values used, i.e. we will create rheological models of AISI-321 steel with a grain size of 700 nm and 200 nm. For the initial grain size, we take the value of 1500 nm, corresponding to the yield strength of 270 MPa, according to equation (1). In [5], extensive studies of the Hall-Petch effect were carried out in relation to the two most used grades of austenitic stainless steels – AISI-316 and AISI-321. As a result, the following values were obtained:  $\sigma_0 = 150 \text{ MPa}$ ;  $k = 420$ . As a result, the following values of the yield strength were obtained:

-  $\sigma_Y = 652 \text{ MPa}$  (for a grain size of 700 nm);

-  $\sigma_Y = 1089 \text{ MPa}$  (for a grain size of 200 nm).

In addition, the second important characteristic required for creating a material rheology is the YS / TS parameter, i.e. the ratio of yield strength to tensile strength. This ratio is not characterized by a linear relationship, but constantly changes depending on the level of deformation and processing conditions of the material. This parameter characterizes the section of the hardening curve between the yield point and the point of failure of the sample. In [12], YS / TS values for AISI-321 steel are presented, as well as data on elongation, on the basis of which the corresponding strength limit values were obtained:

-  $\sigma_{TS} = 986 \text{ MPa}$  (for a grain size of 700 nm);

-  $\sigma_{TS} = 1194 \text{ MPa}$  (for a grain size of 200 nm).

-  $\delta = 38 \%$  (for a grain size of 700 nm);

-  $\delta = 22 \%$  (for a grain size of 200 nm).

After setting these values on the graph as points and processing with the spline function [6], the AISI-321 steel hardening curves were obtained (figure 2a).

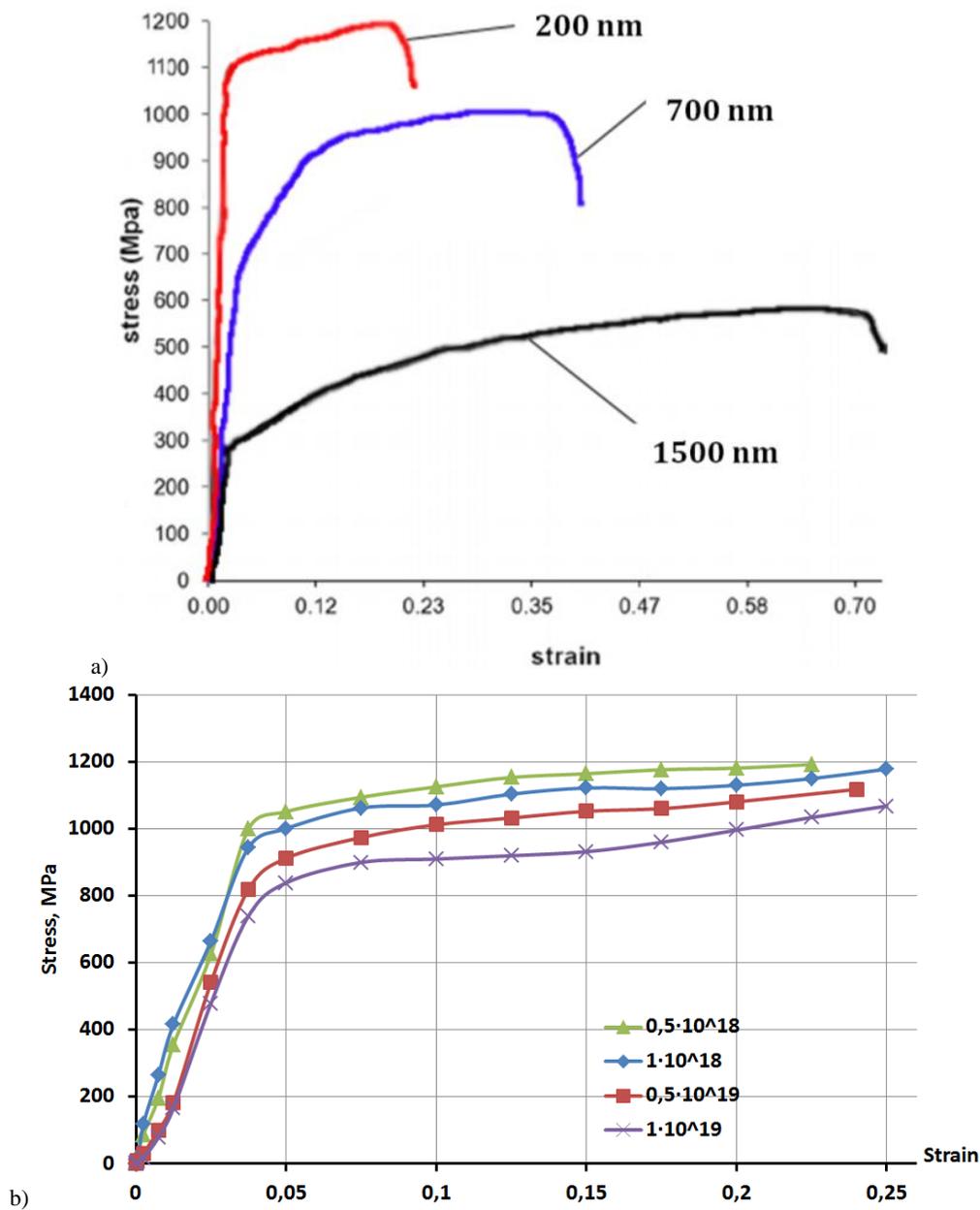


Figure 2 - AISI-321 steel hardening curves for the UFG state

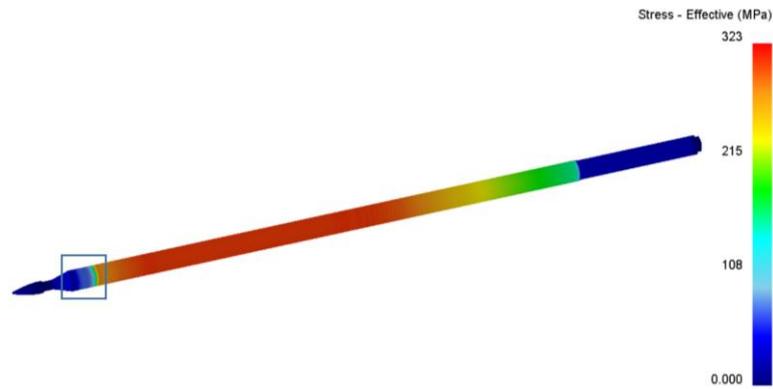
When creating rheological models of irradiated material in the UFG state, the previously discussed method cannot be used. After irradiation, the metal structure is negatively affected by the fast neutron flux. As a result, a partial violation of the crystal lattice occurs at the micro level, which leads to a decrease in mechanical properties. Since it is impossible to predict the level of mechanical properties of such a material using the Hall-Petch equation due to the lack of uniformity of the structure after irradiation, the only possible way to obtain mechanical characteristics here is to conduct plastometric studies.

Plastometric tests were performed using uniaxial compression of cylindrical samples at constant values of the strain rate of  $1 \text{ s}^{-1}$  and a temperature of  $20^\circ\text{C}$ . As a variable parameter, the fast neutron fluence was chosen with the following values:  $0.5 \cdot 10^{18} \text{ n/cm}^2$ ,  $1 \cdot 10^{18} \text{ n/cm}^2$ ,  $0.5 \cdot 10^{19} \text{ n/cm}^2$ ,  $1 \cdot 10^{19} \text{ n/cm}^2$ . The tests were carried out under continuous loading on a Gleeble 3800 plastometric unit using Pocket Jaw module. Based on the test results, graphs of stress-strain flow curves were obtained (figure 2b). The results show that with an increase in the value of fast neutron fluence from  $0.5 \cdot 10^{18} \text{ n/cm}^2$  to  $1 \cdot 10^{19} \text{ n/cm}^2$ , the deformation resistance decreases by about  $\sim 20\%$ , which allows us to conclude that the irradiation has a negligible effect on the properties of AISI-321 steel in UFG state. It should be noted that the deformation resistance of a sample with a

maximum radiation dose of  $1 \cdot 10^{19} \text{ n/cm}^2$  is higher than the properties of a homogeneous UFG material with a grain size of 700 nm. This fact allows us to conclude that, despite the known data on the significant negative impact of radiation on the structure of metals in the usual coarse-grained state, when using materials in the UFG state, the effect of radiation on the structure is significantly reduced.

### 3. Results and discussion

When determining the static load value, the value of 340 MPa was set as the maximum pressure in the core, according to the technical characteristics [1]. The main area of impact of the load on both parts is the central part, while the head and bottom parts serve as retainers. In accordance with this principle, the head and bottom parts were fixed in space on all three axes. After calculating the static load of the fuel Assembly housing, the following results were obtained (figure 3). When analyzing all three models of materials, a similar distribution of stress along the length of the central part of the body of the fuel assembly was noted. Despite the given uniform pressure distribution, the nature of the stress action along the length is uneven and shifted towards the head part.

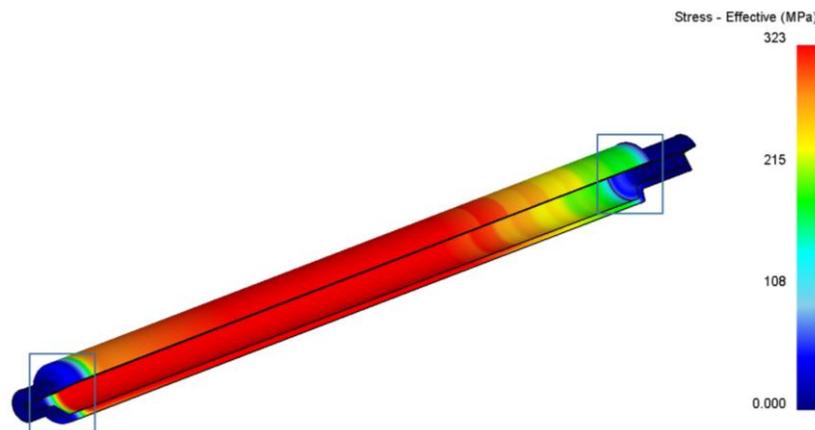


**Figure 3** - Results of calculating the static load of the fuel assembly with a grain size of 1500 nm

Also here, in the area of the junction of the head and central part (in figure 3 this zone is highlighted by a frame), the effect of residual stresses is traced. This phenomenon is a consequence of the design features of the fuel assembly - the head and bottom parts have different lengths, as a result of which different levels of elastic deformation occur in them under static load. The maximum stress value recorded in this model is 274 MPa. According to this value, you can determine the safety margin in the most loaded areas under the specified operating conditions:  $340 \text{ MPa} / 274 \text{ MPa} = 1.24$ .

For the other two models, the following results were obtained: stress in the model with a grain size of 700 nm – 238 MPa; stress in the model with a grain size of 200 nm – 186 MPa; safety margin in the model with a grain size of 700 nm →  $340 \text{ MPa} / 238 \text{ MPa} = 1.43$ ; safety margin in the model with a grain size of 200 nm →  $340 \text{ MPa} / 186 \text{ MPa} = 1.83$ . Thus, when using AISI-321 steel in the UFG state as the fuel assembly material, it is possible to increase the safety margin by 15–47%, depending on the resulting grain size.

After calculating the static load of the fuel element, the following results were obtained (figure 4).



**Figure 4** - Results of calculating the static load of a fuel element with a grain size of 1500 nm

The nature of the stress distribution here is similar to the distribution on the fuel assembly – there is an uneven spread along the length of the central part, with a shift to the head part. However, in contrast to the previously discussed case, in this part, under static load, there are already two centers of action of residual stresses in the areas of the junction of the head and bottom parts with the central one (in figure 4, these zones are highlighted by frames). The presence of such zones at both ends of the central part is a consequence of the fact that the length of the head and bottom parts in the design of the fuel element is not so different as in the case of the fuel assembly.

The maximum values of stresses recorded in these models are as follows: the stress in the model with a grain size of 1500 nm – 313 MPa; the stress in the model with a grain size of 700 nm - 269 MPa; the stress in the model with a grain size of 200 nm – 224 MPa. According to these values, it is possible to determine the safety margin in the most loaded areas for all three materials under the specified operating conditions: the safety margin in the model with a grain size of 1500 nm →  $340 \text{ MPa} / 313 \text{ MPa} = 1.08$ ; the safety margin in the model with a grain size of 700 nm →  $340 \text{ MPa} / 269 \text{ MPa} = 1.26$ ; safety margin in a model with a grain size of 200 nm →  $340 \text{ MPa} / 224 \text{ MPa} = 1.51$ . Thus, when using AISI-321 steel in the UFG state as the material of the body of the fuel element, it is possible to increase the safety margin by 17–40%, depending on the resulting grain size. At the same time, it is necessary to note a decrease in the overall level of safety margin at a constant level of

static load. This phenomenon is directly related to the design features of both parts. In particular, this occurs due to the different wall thickness in the central part – if the wall thickness in the fuel assembly is 4 mm, then in the fuel element it is almost an order of magnitude less – 0.45 mm.

When modeling the behavior of the studied parts made of AISI-321 irradiated UFG steel under static load, the same criteria were used that would be accepted for modeling homogeneous materials. After calculating the static load of the fuel assembly, the following results were obtained:

Maximum stress values:

- in the model after irradiation at  $0.5 \cdot 10^{18} \text{ n/cm}^2$  – 192 MPa;
- in the model after irradiation at  $1 \cdot 10^{18} \text{ n/cm}^2$  - 198 MPa;
- in the model after irradiation at  $0.5 \cdot 10^{19} \text{ n/cm}^2$  - 209 MPa;
- in the model after irradiation at  $1 \cdot 10^{19} \text{ n/cm}^2$  - 227 MPa.

Safety margin for all four irradiated materials under specified operating conditions:

- in the model after irradiation at  $0.5 \cdot 10^{18} \text{ n/cm}^2$  →  $340 \text{ MPa} / 192 \text{ MPa} = 1.77$ ;
- in the model after irradiation at  $1 \cdot 10^{18} \text{ n/cm}^2$  →  $340 \text{ MPa} / 198 \text{ MPa} = 1.71$ ;
- in the model after irradiation at  $0.5 \cdot 10^{19} \text{ n/cm}^2$  →  $340 \text{ MPa} / 209 \text{ MPa} = 1.62$ ;
- in the model after irradiation at  $1 \cdot 10^{19} \text{ n/cm}^2$  →  $340 \text{ MPa} / 227 \text{ MPa} = 1.49$ .

After calculating the static load of the fuel element, the following results were obtained.

Maximum stress values:

- in the model after irradiation at  $0.5 \cdot 10^{18}$  n/cm<sup>2</sup> - 233 MPa;
- in the model after irradiation at  $1 \cdot 10^{18}$  n/cm<sup>2</sup> - 241 MPa;
- in the model after irradiation at  $0.5 \cdot 10^{19}$  n/cm<sup>2</sup> - 249 MPa;
- in the model after irradiation at  $1 \cdot 10^{19}$  n/cm<sup>2</sup> - 258 MPa.

Safety margin:

- in the model after irradiation at  $0.5 \cdot 10^{18}$  n/cm<sup>2</sup> → 340 MPa / 233 MPa = 1.46;

- in the model after irradiation at  $1 \cdot 10^{18}$  n/cm<sup>2</sup> → 340 MPa / 241 MPa = 1.42;

- in the model after irradiation at  $0.5 \cdot 10^{19}$  n/cm<sup>2</sup> → 340 MPa / 249 MPa = 1.37;

- in the model after irradiation at  $1 \cdot 10^{19}$  n/cm<sup>2</sup> → 340 MPa / 258 MPa = 1.31.

Figure 5 shows a summary diagram of the safety factor for the fuel assembly and fuel element when using conventional and irradiated variations of AISI-321 steel in UFG state.

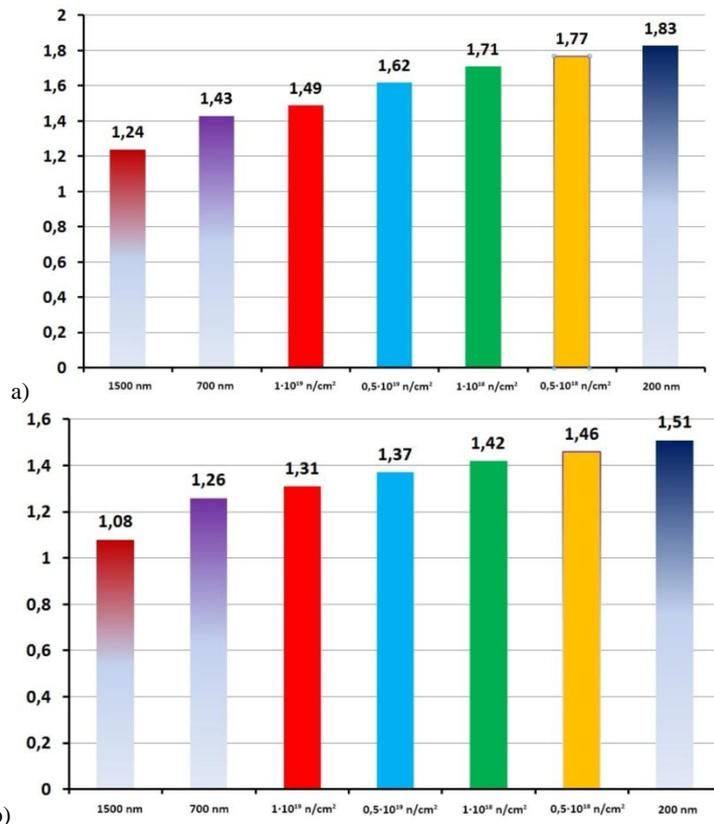


Figure 5 - Diagrams of the safety factor of the fuel assembly (a) and fuel element (b)

Thus, when using AISI-321 steel in the UFG irradiated state as the material both for fuel assembly and fuel element, the margin of safety increases with a decrease in the level of radiation dose. At the same time, it was noted that even at maximum irradiation, the margin of safety in both parts does not reach the lower limit of the UFG structure of 700 nm.

## Conclusions

The creation and calculation of computer models of various products under load with the properties of UFG materials in the normal and irradiated state was carried out. As the products under consideration, the fuel assembly and the fuel element were selected as the most suitable reactor parts in terms of size. To model the properties of UFG non-irradiated AISI-321 steel, the Hall-Petch equation was used to construct hardening curves for the base state of the material at a grain size of 1500 nm and for two UFG states (with grain sizes of 700 and 200 nm). To simulate the properties of UFG irradiated AISI-321 steel, plastometric tests were performed using uniaxial compression of cylindrical samples at constant values of the strain rate of  $1 \text{ s}^{-1}$  and a temperature of 20°C on the "Gleeble 3800" plastometric unit. As a variable parameter, the fast neutron fluence was chosen with the following values:  $0.5 \cdot 10^{18}$  n/cm<sup>2</sup>,  $1 \cdot 10^{18}$  n/cm<sup>2</sup>,  $0.5 \cdot 10^{19}$  n/cm<sup>2</sup>,  $1 \cdot 10^{19}$  n/cm<sup>2</sup>. The maximum operating pressure of 340 MPa was used as a static load. The simulation results showed that for both parts, the use of material in the UFG state is the most appropriate solution, since in this case the margin of safety even

at maximum irradiation in both parts does not reach the lower limit of the UFG structure.

## Acknowledgements

This work was carried out within the framework of the theme № AP05131382 "Development and research of technology for obtaining ultrafine materials with improved mechanical properties and increased radiation resistance for use as materials of the first wall of thermonuclear reactors and in nuclear power" under the grant funding program for scientific and (or) scientific and technical projects for 2018-2020 in the Republic of Kazakhstan.

## References

1. Шмелев В.Д., Драгунов Ю.Г., Денисов В.П., Васильченко И.Н. *Активные зоны ВВЭР для атомных электростанций* (Академкнига, 2004).
2. Shakhova I., Dudko V., Belyakov A., Tsuzaki K., Kaibyshev R. *Mater. Sci. Eng. A* **545** (2012) 176–186.
3. Petch N.J., *J. Iron Steel Inst.* **174** (1953) 25–28.
4. Hall E.O. *Proc. Phys. Soc. Lond. B.* **64** (1951) 747–753.
5. Astafurov S.V., Maier G.G., Melnikov E.V., Moskvina V.A., Panchenko M.Yu., Astafurova E.G. *Mater. Sci. Eng. A* **756** (2019) 365-372.
6. Craven P., Wahba G. *Numerische Mathematik* **31** (1979) 377-403.