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# Modelling of the Zr-2.5Nb alloy properties with hydrides

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## 1. Introduction

The RBMK reactor is designed to use a graphite moderator in the form of graphite bricks which surround zirconium-niobium fuel channels (FC) containing the nuclear fuel and coolant. The fuel channels are initially positioned in place by a series of graphite rings that are alternately in contact with the inner bore hole of the graphite bricks and the outer perimeter of the pressure tubes. The fuel channel is one of the main loop elements of the main circulation circuit. The top, center and bottom segments of typical reactor fuel channels [1] are shown schematically in Fig. 1. The main component of the fuel channel is the coolant carrying tube constructed from separate end and center segments. The center segments (*11*) is an 88 mm outside diameter (4 mm thick wall) tube, made from zirconium-niobium alloy (Zr + 2.5Nb). The top (*9*) and bottom (*15*) segments are made from stainless steel tube. The choise of zirconium-niobium for the center part was made because of relatively low thermal neutron absorption cross-section of the material and its adequate mechanical and anticorrosive properties at high temperatures (up to 350°C). The center and end pieces are joined by special intermediate coupling, made from steel-zirconium alloy.

Fuel channels of RBMK-1500 reactors are the major structural elements of the reactor core therefore it is necessary to evaluate the influence of ageing mechanism on mechanical properties of zirconium-niobium alloys during operation of the reactor. The ageing mechanisms of zirconium tubes are irradiation and thermal creep causing the increase of tube diameter and embrittlement of zirconium alloy under exposure of irradiation and hydrogen absorption. Hydrogen absorbed by zirconium alloy during corrosion process is one of the main factors determining lifetime of Zr-2.5Nb FC. When hydrogen concentration in FC exceeds solubility limit, the formation of hydrides under certain conditions can reduce resistance to brittle fracture and cause the initiation and development of hydride cracks (delayed hydride cracking).

## 2. Modelling of mechanical properties of an alloy with hydrides

The fuel channels are irradiated and experimental investigations for the estimation of the influence of hydrides on mechanical properties of zirconium alloy are complicated. Therefore computational methods for modelling of mechanical properties are import. The finite element method was used for modelling of mechanical properties. The models consist of two materials: Zr_matrix, hydride.

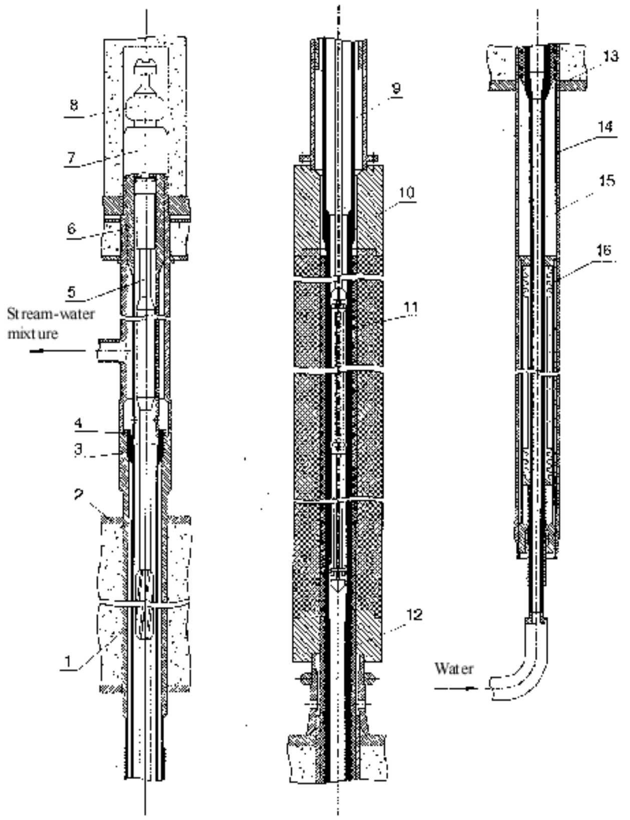



Fig. 1 Fuel channel. *1* - protective screw plug; *2* - structure "E" upper plate; *3* - FC housing in structure "E"; *4* - leak tight weld; *5* - FA suspension unit; *6* - upper FC housing; *7* - FC cartridge; *8* - FC plug; *9* - FC upper part TK; *10* - upper steel-zirconium adapter; *11* - FC middle part; *12* - lower steel-zirconium adapter; *13* - screwed support; *14* - lower FC housing; *15* - FC lower part; *16* - compensating bellow

### 2.1. Alloy matrix mechanical properties

Testing of the zirconium alloy without and with hydrides was performed [2]. The mechanical properties (standard yield strength ($R^T_{p0.2}$ ($\sigma_{0.2}$)), ultimate strength ($R^T_m$ ($\sigma_u$)), ultimate strain ($A$ ($\delta$)), area reduction ($Z$ ($\psi$)) and modulus of elasticity ($E$)) are summarized in Table 1.

An average stress-strain curve (Fig. 2) from tensile testing of the zirconium alloy without hydrides was used in the analysis.

Table 1
Yield strength, ultimate strength, ultimate strain and area reduction of Zr-2.5Nb alloy

| | |
|---|---|
| $R^T{}_m$ ($\sigma_u$), MPa | 492 |
| $R^T{}_{p0.2}$ ($\sigma_{0.2}$), MPa | 411 |
| $A$ ($\delta$), % | 14.78 |
| $Z$ ($\psi$), % | 62.22 |
| $E$, GPa | 34.43 |

2.2. Hydride material properties

Hydride material properties were modelled according the methodology proposed by [3]. The variation of stresses is presented in relation

$$\sigma = \frac{e^2\sigma^2_{max}}{\phi_0}\delta_n \exp\left(-\frac{e\sigma_{max}}{\phi_0}\delta_n\right) \quad (1)$$

here $\sigma_{max}$ is the hydride strength, $\phi_0$ is the work of de-cohesion, $\delta_0$ is normal displacement. Hydride fracture strength $\sigma_{max}$ depends on the modulus of elasticity and is calculated from the relation

$$\sigma_{max} = 7.357*10^{-3}E \quad (2)$$

here $E$ is the elasticity modulus of the hydride obtained from relation

$$E = 95900 - 57.4(T - 273) \quad (3)$$

here $T$ is absolute temperature of alloy, $\phi_0$ is the work of de-cohesion, is calculated from the relation $\phi_0/(\sigma_{max}h)$. This relation values are reported in reference [3]. The $h$ is the length of hydride obtained from experimental investigation (see section 2.3). The $e$ is the base of the natural logarithm.

The calculated stress-strain curve of the hydrides is presented in Fig. 2, which was used in the material properties analysis of zirconium alloy with hydrides.

2.3. Volume part of the hydride clusters in zirconium alloy matrix

The volume part of hydride clusters in the alloy was evaluated by experimental investigation. The obtained results were used for FEM simulation. Also the characteristic dimensions of hydrides were analysed.

The volume part of hydride clusters was found applying the area method [4] in axial-radial (A-R) and radial-transverse (R-T) directions to polished and etched specimens. The examples of hydride cluster morphologies are presented in Fig. 3.

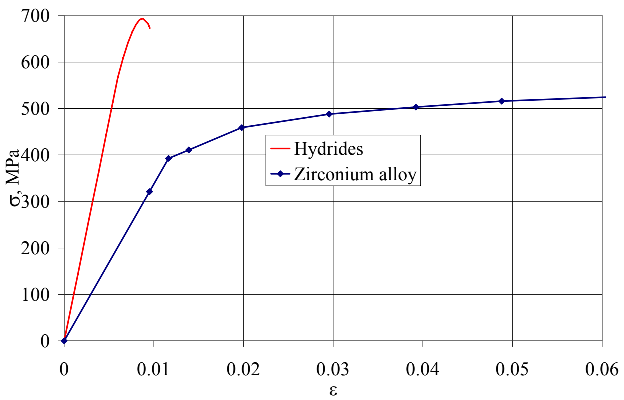
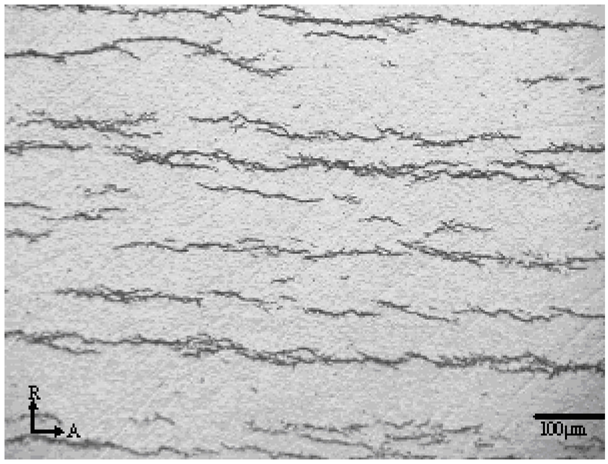
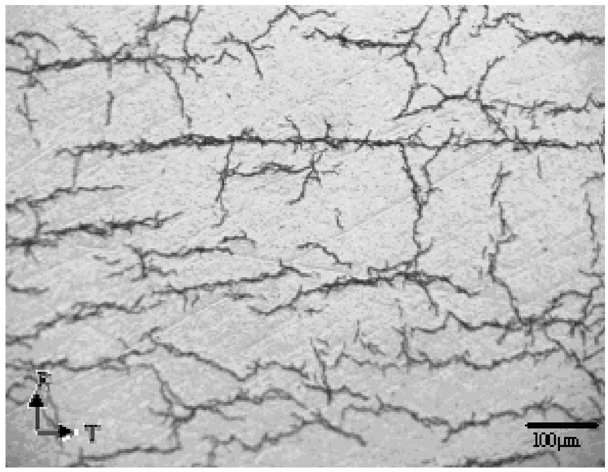



Fig. 2 Stress-strain curves of zirconium alloy without hydrides and hydride at temperature 20°C




a




b

Fig. 3 Hydride distribution in unirradiated RBMK TMT-2 pressure tube material, on the radial – axial (a) and radial – transverse sections (b), at 137 ppm hydrogen concentration

The investigation results of the of volume part of the hydride clusters are presented in Table 2 and Fig. 4. A good coincidence of measurements in A-R and R-T directions was found.

Table 2
Volume part of hydride clusters in Zr-2.5Nb alloy

| Concentration of hydrogen, ppm | Volume of hydrides $V_H$, % | | Mean $V_H$, % |
|---|---|---|---|
| | Section A-R | Section R-T | |
| 23 | 2.4 | 3.0 | 2.7±0.25 |
| 95 | 7.4 | 8.1 | 7.8±0.6 |
| 137 | 10.4 | 9.1 | 9.7±0.8 |
| 360 | 32.0 | 28.6 | 30.3±2.4 |

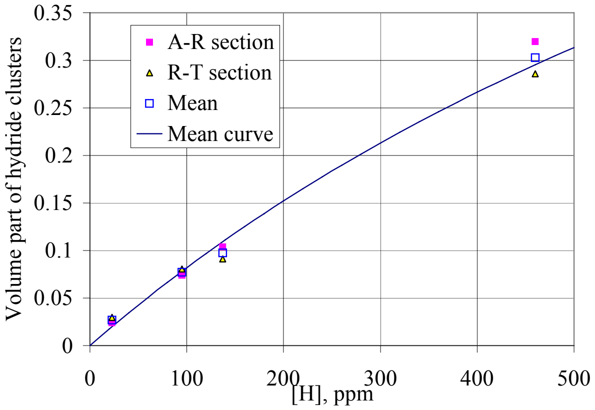



Fig. 4 Variation of the volume part of hydride clusters depending on hydrogen

2.4. FE model of zirconium alloy with hydrides

Modelling of the zirconium alloy with hydrides was performed using finite element method. FE models for the analysis of the zirconium alloy with hydrides were prepared using computer code BRIGADE/Plus [5]. The FE model of the zirconium alloy with hydrides is presented in Fig. 5. This FE model consists of two materials, i.e. zirconium alloy and hydrides. The volume part of hydrides (ZrHx) depending on the concentration of hydrogen is evaluated in this model. The zirconium alloy with hydrides is modelled using the 4-node linear 2D shell elements CPS4 and CPE4 [6]. The CPS4 elements evaluate plane stress condition, i.e. stress in two directions, and strain in three directions. The CPE4 elements evaluate plane strain condition, i.e. strain in two directions, and stress in three directions. CPS4 elements were used for stress – strain diagram modelling in elastic part, and CPE4 – plastic part. The displacement load was used in stress-strain diagram modelling.

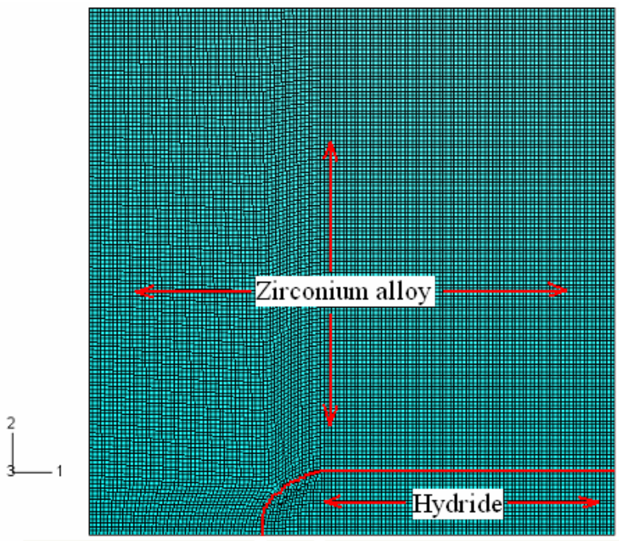



Fig. 5 FE model of zirconium alloy with hydrides

2.4. Results of mechanical properties modelling

The aim of stress analysis of the zirconium alloy with hydrides was to calculate stress – strain relationships depending on hydrogen concentration. The prognoses of stress – strain curves of zirconium alloy with different hydrogen concentration were performed at the temperature 20°C. The static analysis was performed using the BRIGADE/Plus code. The analysis results are presented as stress snapshots in Fig. 6. Fracture of the specimen is beginning in hydride inclusion when strength limit of the hydride, i.e. 630 MPa is exceeded.

The analysis results in case of hydrogen concentration 100 ppm is presented in Fig. 7. The prognosis results were compared with experimental data. Good coincidence of the prognosis results with the experimental data was received. The deviation of the modelled stress – strain curve from experimental does not exceed 1 %. The stress – strain curve of the zirconium alloy is presented in this picture. It is seen that zirconium alloy strengthening depends on hydride concentration.

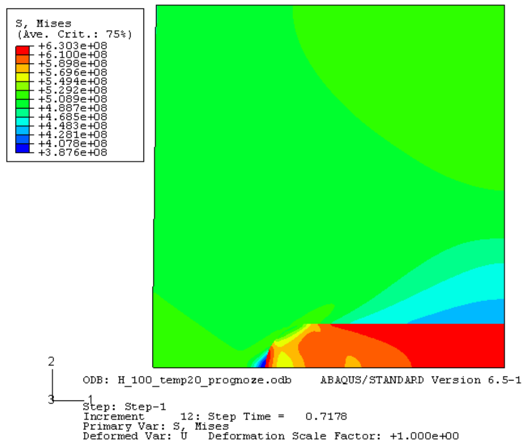



Fig. 6 Von Misses stress (Pa) distribution of the zirconium alloy with hydrides at the temperature 20°C

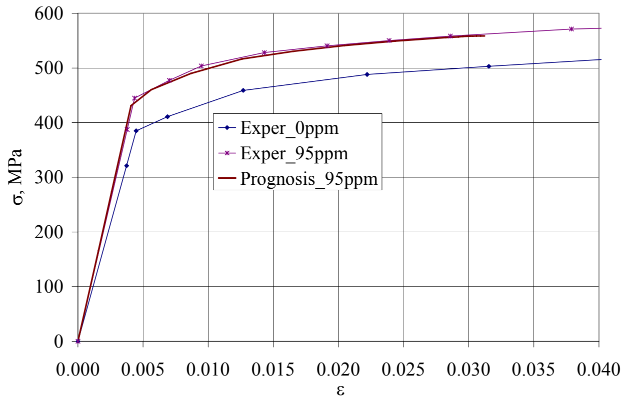



Fig. 7 The experimental and modelled stress strain curve of zirconium alloy with hydrogen concentration 100 ppm at the temperature 20°C

## 3. Summary and conclusions

The modelling of material properties of the zirconium - niobium alloy (Zr-2.5Nb) with hydrides was performed using finite element method. The FE model used for this analysis consists of two materials, i.e. zirconium niobium alloy and hydrides. The volume part of hydrides depending on hydrogen concentration is evaluated in this model. The tested material properties of zirconium alloy and the calculated properties of the hydrides were used in these analyses.

Comparison of the prognoses results of mechanical properties of zirconium alloy without and with hydrides and experimental data show that the deviation of the modelled stress – strain curve from the experimental does not exceed 1 %. These results permit the statement that the FE method can be used for the modelling of material properties of the zirconium - niobium alloy with hydrides.

**Acknowledgments**

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Zr-2,5Nb LYDINIO SU HIDRIDAIS SAVYBIŲ MODELIAVIMAS

R e z i u m ė

Reaktoriaus RBMK-1500 kuro kanalai yra vienas iš svarbiausių reaktoriaus struktūrinių elementų. Kuro kanalų, pagamintų iš Zr–2,5Nb lydinio, ilgaamžiškumui turi įtakos korozija ir korozijos proceso metu ištirpęs vandenilis. Todėl svarbu nustatyti hidridų poveikį cirkonio lydinio savybėms.

Hidridų poveikio Zr–2.5Nb lydinio savybėms modeliavimas atliktas taikant baigtinių elementų metodiką. Esant skirtingai vandenilio koncentracijai, hidridų klasterių tūrinė dalis lydinio matricoje įvertinta remiantis metalografiniais tyrimais. Prognozavimo rezultatai palyginti su eksperimentiškai nustatytais duomenimis. Tyrimų rezultatai parodė, kad baigtinių elementų metodas gali būti taikomas kanalų mechaninėms charakteristikoms modeliuoti atsižvelgiant į hidridinės fazės kiekį cirkonio lydinio matricoje.

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MODELLING OF THE ZR-2.5NB ALLOY PROPERTIES WITH HYDRIDES

S u m m a r y

Fuel channels of RBMK-1500 reactors are the major structural elements of the reactor core. Hydrogen absorbed by zirconium alloy during corrosion process is one of the main factors determining lifetime of Zr-2.5Nb FC. Therefore the evaluation of the influence of hydrides on fracture parameters of zirconium alloy is important.

The volume part of the hydrides at different hydrogen concentration was evaluated. The volume of the hydrides was specified from metallographic investigation. The modelling of the influence of hydrides on mechanical properties of zirconium-2.5niobium alloy was performed using finite element method. The prognosis results were compared with the experimental data. The results of investigations demonstrated that the Finite Element method could be used for the modelling of material properties of fuel channels.

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МОДЕЛИРОВАНИЕ СВОЙСТВ ZR –2.5NB С ГИДРИДАМИ

Р е з ю м е

Технологические каналы реактора РБМК-1500 являются одним из основных структурных элементов реактора. На долговечность технологических каналов, изготовленных из сплава Zr-2.5Nb, влияет водород, который в процессе коррозии в нем растворяется. Поэтому важно оценить влияние гидридов на свойства сплава циркония.

Моделирование влияния гидридов на свойства сплава Zr–2.5Nb выполнено используя метод конечных элементов. При разной концентрации водорода объемная доля гидридных кластеров в матрице сплава определена используя методы металлографического анализа. Результаты прогноза расчетов сравнены с экспериментально установленными данными. Полученные результаты исследования показали, что метод конечных элементов может быть использован для моделирования механических характеристик технологических каналов с учетом количества гидридной фазы в матрице циркониевого сплава.

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