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Simulation of Point Defects Formation in the Fuel Element of a Nuclear Power Plant's Wave Reactor

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Abstract. This paper considers the point defects that influence the operation of a wav nuclear power reactor with a uranium fuel medium. The formed individual point defects or such defect groups can produce a perturbing effect on the stability of the nuclear reactor operating mode and involve its transition to an unstable state. Studies have been carried out on the effect on the characteristics of the nuclear burnup wave in a medium with neutron multiplication for 2D geometry. For the calculation, the uranium-thorium fissile medium has been considered. The parametric calculations were carried out with ^{235}U different enrichment percents and different values of neutron activation energy. At that, it was assumed that the wave (flow) reactor stable operation region is located in the range of activation energies from 10^{-3} eV to 1 eV or in the region from 2 MeV to 8 MeV. When calculating the neutron flux intensity in a wave reactor, the influence of point defects and their aggregates on the decelerating elastically scattered neutrons' flux density and the flux density of decelerating non-elastically scattered neutrons was considered. The dependences of the point defects formation rate on the medium fissile temperature for several compositions of the uranium-thorium medium are obtained. As visually identified, the graphic materials obtained during the calculations are similar to the photos of fuel rods after the energy campaign.

Keywords: process visualization, defects spatial distribution, fuel rod damage mechanism, process innovation.

1 Introduction

This article continues the study of the theoretical mechanism for defects in spatial distribution. The given study includes numerical modeling on that mechanism basis and the obtained graphic material.

The study's relevance is determined by identifying the fuel assembly state and main behavior patterns, depending on the damaging nature and the operation duration.

This study aims to verify the results of calculations by the proposed mechanism on the material of fuel assembly cuts after the fuel campaign on actually operating power plants.

One of the reasons for the disturbing effect on the nuclear reactor operating mode stability and the decrease in the NPPs installed power factor (IPF) is the formation of defects in fuel elements of various reactors [1, 2].

The processes of the appearance of defects, depending on the processes occurring in fuel during the reactor operation, are considered in [3].

The dynamic aspects of forming point defects of the type substitution and intrusion during reactor operation are considered in [4, 5].

In most cases, the reason for the installed power factor (IPF) relatively low values is the static occurrence of damage to fuel assemblies (FA) through the formation of a defect in the fuel cladding [1].

Based on the results in the field of irradiated fuel assemblies post-reactor examinations [6-8], also taking into account the materials of defects study in the early stages of nuclear energy industry development [9-11], it should be noted that the main mechanisms of damage to fuel rods due to radiation growth, thermomechanical interaction between fuel and cladding, radiation and thermal creep, deflection of fuel rods (associated with

thermomechanical interaction in the bundle), and radiation-resulting decrease in plasticity.

2 Research Methodology

Due to the processes of heat intake and heat removal from the system to the medium, the reactor heating and the change in fuel component concentration are described by the following system of equations [4]:

$$\frac{dT}{dt} = \Phi\frac{Qpc}{c_p m}e^{\frac{-E}{RT}} - a(T - T_\infty)S; \quad (1)$$

$$\frac{dC}{dt} = \frac{u}{V}(C_0 - C) - ze^{\frac{-E}{RT}}C, \quad (2)$$

where Q – the thermal reaction effect; $\Phi = \Phi(E)$ – the rate of particle generation in the reaction; p – the reacting medium density; C_0, C – the initial and current concentrations of the fuel component, respectively; E – the activation energy, i.e., the energy that the neutron must have to react; T – reactor temperature; α – the heat transfer coefficient; T_∞ – the ambient temperature; V – the volume in which the reaction takes place; S – the surface area limiting the volume; c_p – the specific heat capacity at constant pressure; m – the reacting system mass; u – the burning nuclear fuel wave speed, or the rate of nuclear fuel components supply (in the case of a flow reactor).

It is known from previous works [12–14] that an appropriate equation also describes the neutron flux intensity in wave reactor temperature dynamics:

$$\Phi(E) = \Phi_1(E) + \Phi_2(E), \quad (3)$$

where $\Phi_1(E)$ – an expression for the flux density of decelerating elastically scattered neutrons; $\Phi_2(E)$ – an expression for the flux density of decelerating non-elastically scattered neutrons.

The PD concentration in the sample depends on spatial coordinates and time [3]. Therefore, it can be found from the solution of a system of two diffusion equations describing the migration of PD, which closes the general system of equations (1)-(5):

$$\frac{\partial C_V(r,t)}{\partial t} + \omega\nabla\vec{J}_V(\vec{r},t) = -\alpha C_V(\vec{r},t)C_I(\vec{r},t); \quad (4)$$

$$\frac{\partial C_I(r,t)}{\partial t} + \omega\nabla\vec{J}_I(\vec{r},t) = -\alpha C_V(\vec{r},t)C_I(\vec{r},t), \quad (5)$$

where $C_V(r,t)$, $C_I(r,t)$ – the concentrations of vacancies and interstitial atoms, respectively; $J_V(r,t)$ and $J_I(r,t)$ – the flux densities of vacancies and interstitial atoms; $\omega \sim \alpha^3$ – the atomic volume; a – the lattice constant; α – the PD mutual recombination coefficient.

Since the PD sources density is proportional to the rate of nuclear fission or the neutron flux density, considering the neutron capture cross-section (3).

Then, estimated computer calculations of the PD sources' density dependences on temperature can be carried out for several compositions, for example, a uranium-thorium fissile medium at a constant neutron flux density; the results are shown in Figure 1.

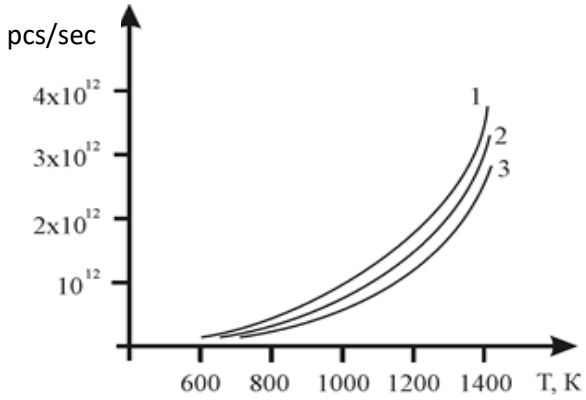

Figure 1 – Dependences of the rate of point defects formation on the medium fissile temperature for several compositions of the uranium-thorium medium (1-10 % Th; 2-5% Th; 3-1% Th) at a constant neutron flux density $F = 10^{13}$ neutrons/(cm^2·s)

Calculations were carried out for the wave (flow) reactor stable operation region, presumably located from 10^{-3} eV to 1 eV or in the region from 2 MeV to 8 MeV.

When simulation, we use the following initial data:

$E_u = 5{,}5\ MeV = 5{,}5 \cdot 10^6 \cdot 1{,}6 \cdot 10^{-19}\ C = 8{,}8 \cdot 10^{-13}\ J$;
$E_{Th} = 5{,}9\ MeV = 5{,}9 \cdot 10^6 \cdot 1{,}6 \cdot 10^{-19}\ C = 9{,}44 \cdot 10^{-13}\ J$;
$Q_u = 204\ MeV = 204 \cdot 10^6 \cdot 1{,}6 \cdot 10^{-19}\ C = 326{,}4 \cdot 10^{-13}\ J$;
$Q_{Th} = 190\ MeV = 190 \cdot 10^6 \cdot 1{,}6 \cdot 10^{-19}\ C = 304 \cdot 10^{-13}\ J$.

The calculations assumed that the thorium-specific heat capacity coincides with uranium's specific heat capacity.

It should be noted that the solution of this equations' system is associated with overcoming large computational difficulties due to the need to set boundary conditions on all PD drains, which, as a rule, are chaotically distributed over the sample volume. During the numerical simulation, these processes were not considered.

3 Results and Discussion

Later, an attempt was made to visualize the PD formation process. During the simulation, we considered the physical parameters of fuel energy-emitting elements' tablets (fuel elements) manufactured by powder metallurgy technology and their isotopic composition. The simulation was carried out according to such parameters as the total neutron flux, the point defects migration distance, and the size of a cell containing the active isotope. The simulation results are presented in a series of Figures 2-5 obtained using computer models.

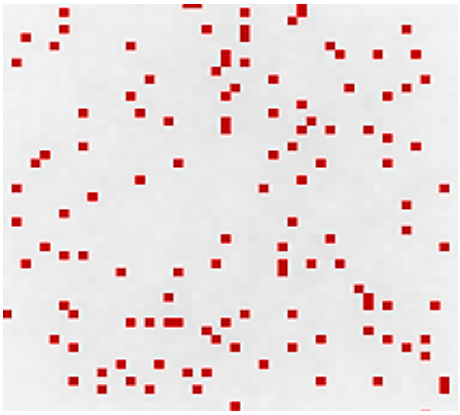

Figure 2 – Simulation of 2D chaotic placement of cells with an active isotope in a model fuel element (simulation size 6000×6000 μm), the beginning of calculations; the active isotope containing cell size (highlighted in red) is ~100 μm per cell

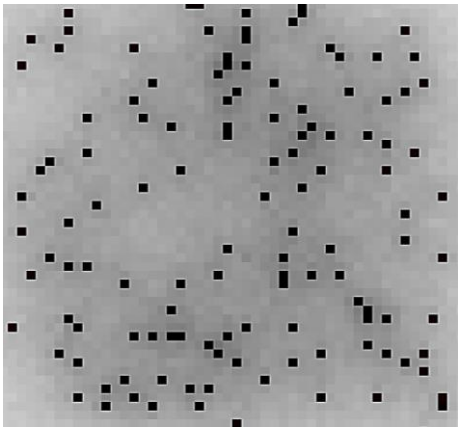

Figure 3 – Simulation of 2D chaotic placement of point defects (different grayscale) in a model fuel element (simulation size 6000×6000 μm), end of calculations

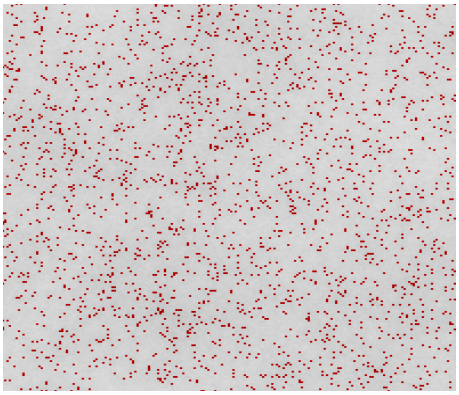

Figure 4 – Simulation of 2D chaotic placement of cells with an active isotope in a model fuel element (simulation size 200×200 μm, the beginning of calculations; the active isotope containing cell size (highlighted in red) is ~1 μm per cell)

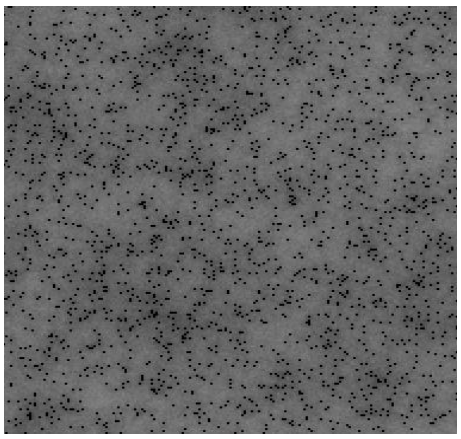

Figure 5 – Simulation of 2D chaotic placement of point defects (different grayscale) in a model fuel element (simulation size 200×200 μm, end of calculations; the active isotope containing cell size (highlighted in black) is ~1 μm per cell

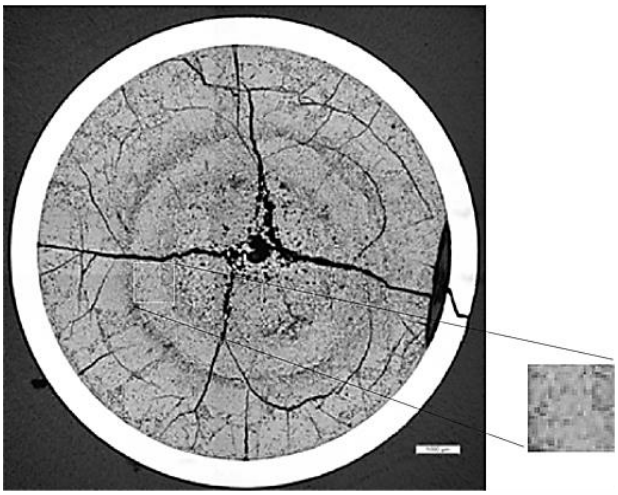

Figure 6 – Photo of the fuel rod after the fuel campaign (1), the same fuel element photo fragment, magnification by 10 (2); the results obtained allow us to state the correctness of the methodological and theoretical approach in modeling

It should be noted separately that the fuel tablet swelling and cracking processes were not considered in the simulation. These studies will be carried out further in the future.

Analysis of photos of fuel rods after the fuel campaign (Figure 6) showed their visual similarity with the graphic material obtained from numerical simulation carried out in the presented work (Figure 6 and, for example, Figure 5).

4 Conclusions

As a result of the research work carried out, the following conclusions are formulated.

The point defects influencing the wave (flow) reactor operation with uranium-thorium fuel medium are considered. As a result of numerical simulation, the dependences of the point defects formation rate on temperature are obtained. These dependencies are power functions of temperature with an exponent equal to 4.

Numerical modeling was carried out, with calculation results visualization, the processes of a chaotic PD region formation, with a variation in the size of active isotope-bearing cells, from 1 μm to 100 μm per cell.

The resulting graphic material of 2D modeling of point defects formation is visually similar to photographs of fuel element (TVEL) sections after the fuel campaign (excluding cracking and swelling).

The carried out visual similarity confirms the correctness of the theoretical approach applied in numerical modeling and allows for developing software for these processes simulation.

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