SIMULATION OF THE RADIATION CREEP OF A REACTOR FUEL

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Are submitted the computer system for radiation creep simulation, developed on the basis of the offered model of a radiation creep and the method of dynamic simulation of a dislocation movement, and results of computer experiment on radiation creep research on an example of technical uranium and its alloys with the small additions of molybdenum (0,9 % ÷ 1,3 %).

1. INTRODUCTION

The special interest represents study of a radiation creep of materials. The majority of experimental data on radiation creep concerns to already used in working reactors materials, which were tested in conditions close to working modes of reactors. The experimental researches of radiation damage of materials and change of their properties are connected to the large expenses of work, means and time, and also frequently with significant difficulties of technical and technological character. The large variety of theoretical models of radiation creep is united by one common parcel - presence in an irradiated material of high concentration of point defects (PD) and sinks for them. The account of this parcel with attraction of dislocation representations allows to explain features of radiation creep of materials under a loadings by result of gliding and climbing of dislocations in a field of the distributed obstacles. The theoretical models, constructed on the basis of these representations and using the analytical description, allow to receive analytical expressions for speed of radiation creep, allowing qualitatively to judge character of influence of some factors on radiation creep rate. However quantitative revealing of features of radiation creep on the basis of model of dislocation movement in a field of the distributed obstacles is possible only with attraction of methods of mathematical simulation on a computer. Therefore special value is represented by development of computer systems for radiation creep simulation, allowing to receive estimations of radiation creep speed in significant ranges of change of such parameters, as temperature, loading and density of a radiation flow.

The computer simulation of nuclear structures of defects in crystals and their reorganizations under influence of loadings, thermal fluctuations and irradiation became the important method of research. The authors [1] consider, that the time comes nearer, when the statement anyone (especially expensive) experiment in radiation physics will be preceded by its computer simulation. Many models of computer simulation of radiation defects allowing are nowadays known to find in this or that approximation types of defective structures. Clearly, however, that the finding of defective structures, that is finding of distributions in space of a various sort of defects of a crystal lattice, is only first step of research. Its following step should consist in study of influence of all set of defects on change of those or other physical properties of metals at an irradiation. The development of computer simulation of radiation damages, as was emphasized in [2], is connected to development of complex computer simulation systems, which will unite in themselves various more private algorithms of simulation of nuclear structures of defects in crystals and their reorganization. Preliminary structure of such system submitted in a fig.1 there was discussed.

The development of ideal computer system for radiation creep simulation demands development of complex simulation system, which structure will be coordinated to structure submitted on a fig. 1. However development of such system while remains by affair of the future. Today efforts are concentrated on development simplified simulation radiation creep system, which main component is the system of dislocation movement simulation, for which work all other necessary making (fig. 1) are set as entrance parameters, for with the help of such systems it is possible to receive estimations of radiation creep speed. In the future the developed simulating systems of dislocation movement will enter by a key part in ideal computer system simulating radiation creep of materials.

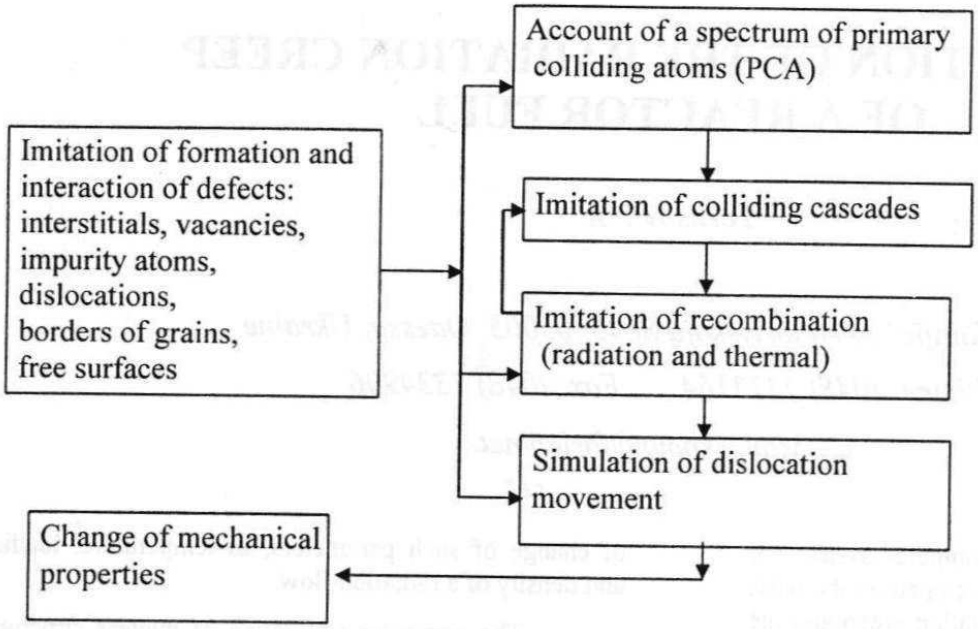

Fig. 1. The structure of system simulating influence of an irradiation on mechanical properties.

2. PHYSICAL MODEL OF RADIATION CREEP

The physical model accepted by the author, assumes presence in an irradiated material active to movement dislocations, obstacles for driving dislocations, as which the spherical centers of expansion of various capacity and dislocation loops of a edge type were considered, and PD (interstitials and the vacancies), generated by an irradiation (in divided materials PD are generated also by process of braking of splinters of division), and the established concentration PD considerably exceeds thermoequilibrium. The model of a radiation creep is explained within the framework of the mechanism of gliding and climbing dislocations based on the conception of a dislocation as not ideal sink for PD [3]. The model is efficient for installed concentration PD, considerably exceeding thermally steady state concentration. The gliding of dislocation are describing as due to moving dislocation kinks in Peierl's relief. The climbing of dislocation are describing as due to moving dislocation jogs.

3. METHOD OF DYNAMIC SIMULATION OF FLEXIBLE DISLOCATIONS MOVING

The mathematical model of dislocation movement is based on model of dislocation gliding in a Peierl's relief, carried out by means of movement of kinks, and on model of dislocation climbing carried out by means of movement of dislocation jogs being sinks for PD [3]. The obstacles are described by the fields of stress, for example. voids, spherical congestions of point defects, spherical allocation in alloys and, under certain conditions, admixture atoms in solid solutions of replacement, and also the introduced splinters of divided materials are described by a stress field of a spherical-symmetric center of expansion.

According to a method of dynamic simulation of dislocations movement mathematical simulation on the computer of gliding and climbing of flexible dislocation was carried out as follows. On a dislocation line gets out N of basic points (each point there corresponds an elementary segment of a dislocation line), the movement by each of which pays off according to the equations of the following system:

$$(\vec{V},\vec{\xi})=0,$$

$$(\vec{V},\vec{n}_{gl})=A_1\left|d\vec{F}_{el}\right|\left(\text{sign}\left\{d\vec{F}_{fr}-(d\vec{F}_{el},\vec{n}_{gl})\right\}-1\right), \quad (1)$$

$$(\vec{V},\vec{n}_{cl})=A_2^I(d\vec{F}_{el}+\vec{F}^I_{con},\vec{n}_{cl})-A_2^V(d\vec{F}_{el}+\vec{F}^V_{con},\vec{n}_{cl}),$$

where $\vec{V}$ - speed of movement of a basic dislocation point, $\vec{\xi}$ - unit tangent vector of a dislocation line, $\vec{n}_{gl}$ - unit vector determining a direction of gliding, $\vec{n}_{cl}$ - unit vector determining a direction of climbing, $d\vec{F}_{el}$ - force caused by elastic stress fields (a stress of external loading, a stress of obstacles, a stress of dislocation self-action), $d\vec{F}_{fr}$ - force of friction determined by a starting stress of dislocation, A_1-coefficient, the meaning for which can be received from expression for speed of gliding dislocation, A_2^α - the coefficients, the meanings for which can be received from expression for speed of climbing dislocation, $\vec{F}^\alpha_{con}$ - concentration forces caused by superfluous concentration of PD [3].

The equation system (1) is adhered to local system of coordinates, formed by vectors $\vec{\xi}, \vec{n}_{gl}, \vec{n}_{cl}$, and at movement of flexible dislocation these vectors can change the direction, therefore in common system of coordinates the making speeds of movement of a basic point are defined by the following expression

$$V_i' = \ell_{ij} V_j , \qquad i, j = 1,2,3, \qquad (2)$$

where V_j - are calculated on the equations (1), ℓ_{ij} - cosines of angles between axes of local and common systems of coordinates. The location of a basic point "n" in common system of coordinates through k- steps of account is defined by expression

$$(x_i^n)^k = (x_i^n)^{k-1} + (V_i'^n)^k \cdot \tau , \text{ where } i = 1,2,3. \quad (3)$$

The location of a dislocation line is defined by means of approximation of the locations of basic points. At realization of simulating accounts it was considered, that at the initial moment of time dislocation is rectilinear and has edge character, that the boundary points of a dislocation line are so removed from obstacles, that the direction of a dislocation line in these points remains constant.

4. COMPUTER SYSTEM, SIMULATING OF A RADIATION CREEP, AND RESULTS OF SIMULATION

The computer system simulating of radiation creep of the block of a model crystal, taking place under action of stretching loading, is developed, according to above described theoretical model of radiation creep and method of dynamic simulation of gliding and climbing dislocations. It is considered, that in the block of a model crystal a planes of active dislocation gliding are focused in relation to the enclosed external loading according to angle $\lambda = 45^\circ$ and active dislocations, which movement is simulated and also which movement causes creep, rely originally rectilinear and parallel to an axis OX_1.

Agrees [4] creep rate of the simulated block of a crystal is estimated according to expression

$$\dot{\varepsilon} = b\rho u^* , \qquad (4)$$

where $$u^* = \frac{1}{\Delta\tau \rho V} \sum_i^N \Delta S_i , \quad (5)$$

ρ - density of mobile dislocations, b - module of a Burger's vector, ΔS_i - area, covered i dislocation in time $\Delta\tau$, V - volume of a crystal, N - number of dislocations in volume V.

As obstacles were considered spherical centers of expansion and edge dislocation loops (simulates of a prismatic dislocation loop both interstitial and vacancy type formed in a plenty in uranium at an irradiation).

The account of stress (external stress, stress of the spherical center of expansion, stress of a dislocation loop, stress of dislocation self-action) is carried out in elastic continuum approach.

At realization the computer experiments on radiation creep research for the block of a modeling crystal the parameter of a crystal lattice, size of atom, coefficients of diffusion, characteristics and other parameters, which task is necessary for modeling were set appropriate for uranium. Let's result some of them: $\mu = 7{,}05 \cdot 10^{10}$ N/m^2, $\nu = 0{,}35$, radius of atom $r_a = 1{,}41 \cdot 10^{-10}$ m, Burger's vector of dislocation $b = 2{,}5 \cdot 10^{-10}$m, dislocation density $\rho \sim 10^{13}$ m^{-2}, formation energies of vacancy and interstitial accordingly - $F_V \approx 2 \cdot 10^{-19}$ J and $F_I \approx 5 \cdot 10^{-19}$ J, formation energy of a dislocation kink $F_K \approx 1 \cdot 10^{-19}$ J, formation energy of $F_{jog} \approx 1 \cdot 10^{-19}$ J. In a wide range of temperatures active dislocation, ensuring deformation of uranium, are dislocations, having a Burger's vector in direction [110] and system of sliding (010) [110].

At realization the computer experiments on radiation creep research of technical uranium and its alloys with the small additions of molybdenum (from 0,9 % up to 1,3 %) the following results are received. The received dependence of the established radiation creep rate of technical uranium from external loading has linear character and is in the good consent with experimental data [5]. The dependence of the established radiation creep rate of technical uranium from interstitial concentration is received. As the interstitial concentration is proportional to density of a neutrons flow, the comparative analysis of the submitted curve and experimental dependence of established radiation creep rate of technical uranium from density of a flow of neutrons is competent [5]. The comparative analysis shows that settlement and experimental dependence qualitatively and quantitatively are coordinated among themselves [5]. Comparison of the received results and experimental data also allows to make a conclusion that the established interstitial concentration in uranium at density of a flow $\sim 10^{12}$ n/cm^{2}s is in an interval $10^{-11} \div 10^{-13}$.

In the fig.2 the curve of dependence of the established radiation creep rate from temperature for the technical uranium received as a result of simulating accounts at loading $\sim 1 \cdot 10^7$ N/m^2 and established interstitial concentration$\sim 10^{-12}$ is submitted. In the fig.2 the curve of dependence of the established radiation creep rate from temperature for alloys of uranium with the small additions of molybdenum (0,9%÷1,3 %), received as a result of simulating accounts at loading

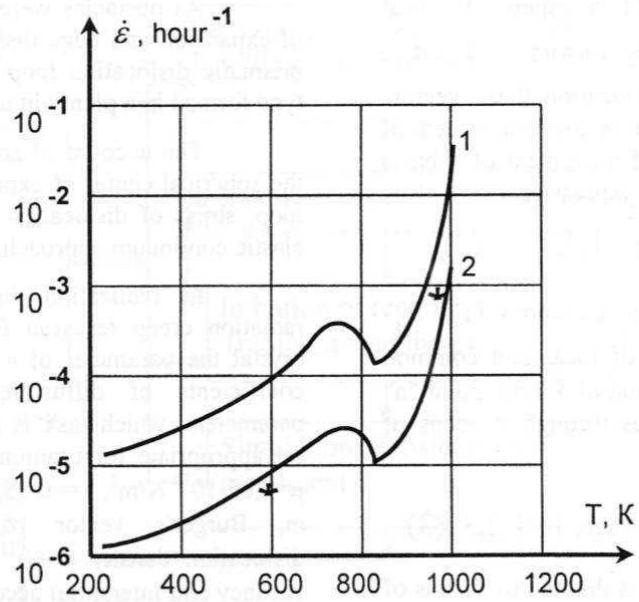

Fig. 2. The temperature dependencies of the established radiation creep rate $\dot{\varepsilon}$ for the technical uranium (curve 1) and for alloys of uranium with the small additions of molybdenum (0,9%÷1,3 %) (curve 2) at neutron flow density $\sim 10^{12}$ n/cm^{2}s and loading $\sim 1 \cdot 10^7$ N/m^2, where T - temperature (* - experimental meanings [6, 7]).

$\sim 1 \cdot 10^7$ N/m^2 and established interstitial concentration $\sim 10^{-13}$, is also submitted. At construction of a curve the experimental data given in works [6, 7] were taken into account and marked on figure by asterisks.

5. CONCLUSION

The computer system for radiation creep simulation, developed on the basis of radiation creep model, considering gliding and climbing dislocations as a not ideal sink for PD, and method of dynamic modeling of dislocations movement, is submitted.

The results of computer experiment on radiation creep of technical uranium and its alloys with the small additions of molybdenum (from 0,9 % up to 1,3 %) are received.

Are submitted the curve of dependence of the established radiation creep rate from temperature for the technical uranium and the curve of dependence of the established radiation creep rate from temperature for alloys of uranium with the small additions of molybdenum (0,9%÷1,3 %), received as a result of simulating accounts. The submitted curves allow to predict temperature behavior of uranium and its alloys and having practical importance for successful designing of reactor elements, their safe operation and forecasting of their behavior in emergencies.

The received results show that the developed computer system is effective addition to direct experimental researches.

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